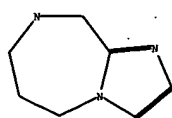
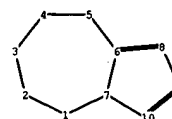


(Untitled)



L19



ring nodes :

1 2 3 4 5 6 7 8 9 10

ring bonds :

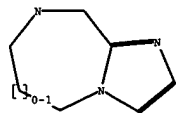
1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

exact/norm bonds :

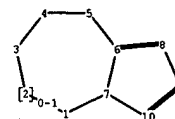
1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom



13



L23

ring nodes :

1 2 3 4 5 6 7 8 9 10

ring/chain nodes :

13

ring bonds :

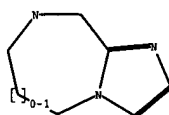
1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

exact/norm bonds :

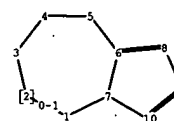
1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 13:CLASS



L2



ring nodes :

1 2 3 4 5 6 7 8 9 10

ring bonds :

1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

exact/norm bonds :

1-2 1-7 2-3 3-4 4-5 5-6 6-7 6-8 7-10 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom

09/868,356

=> d his

(FILE 'HOME' ENTERED AT 15:46:10 ON 01 JUL 2003)

FILE 'REGISTRY' ENTERED AT 15:46:20 ON 01 JUL 2003

L1 STRUCTURE UPLOADED
L2 QUE L1
L3 25 S L2
L4 1302 S L2 SSS FUL

FILE 'CAPLUS' ENTERED AT 15:47:10 ON 01 JUL 2003

L5 256 S L4
L6 ANALYZE L5 1- RN HIT : 1208 TERMS

FILE 'REGISTRY' ENTERED AT 15:47:52 ON 01 JUL 2003

L7 1 S 14483-72-8/RN
L8 1 S 64738-53-0/RN
L9 1 S 78105-31-4/RN
L10 1 S 91476-80-1/RN
L11 1 S 97420-76-3/RN
L12 100 S 68009?/RN

FILE 'CAPLUS' ENTERED AT 15:49:31 ON 01 JUL 2003

L13 1 S WO200039130/PN
SELECT RN L13 1-

FILE 'REGISTRY' ENTERED AT 15:49:56 ON 01 JUL 2003

L14 148 S E1-148
L15 80 S L4 AND L14

FILE 'CAPLUS' ENTERED AT 15:51:39 ON 01 JUL 2003

L16 6 S L15

FILE 'REGISTRY' ENTERED AT 15:51:49 ON 01 JUL 2003

L17 38 S L12 AND L4
L18 STRUCTURE UPLOADED
L19 QUE L18
L20 306 S L19 SUB=L4 FUL

FILE 'CAPLUS' ENTERED AT 15:57:24 ON 01 JUL 2003

L21 70 S L20

FILE 'REGISTRY' ENTERED AT 15:58:15 ON 01 JUL 2003

L22 STRUCTURE UPLOADED
L23 QUE L22
L24 905 S L23 SUB=L4 FUL
L25 233 S L20 AND L24
L26 73 S L20 NOT L25

FILE 'CAPLUS' ENTERED AT 15:59:48 ON 01 JUL 2003

L27 46 S L25

=> s 124

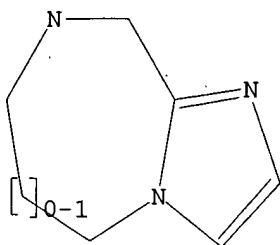
L28 200 L24

=> d 123

L23 HAS NO ANSWERS
L22 STR

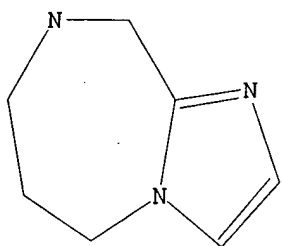
09/868,356

N



Structure attributes must be viewed using STN Express query preparation.
L23 QUE ABB=ON PLU=ON L22

=> d 119
L19 HAS NO ANSWERS
L18 STR



Structure attributes must be viewed using STN Express query preparation.
L19 QUE ABB=ON PLU=ON L18

=> d bib abs hitstr 127 1-46

~~127~~ ANSWER 1 OF 46 CAPLUS COPYRIGHT 2003 ACS

~~AN~~ 2003:173578 CAPLUS

DN 138:221605

TI Preparation of tricyclic pyridin-2-one analogues as ligands for GABAA receptors

IN Bourrain, Sylvie; Goodacre, Simon Charles; Hallett, David James; Lewis, Richard Thomas; Rowley, Michael; Sternfeld, Francine; Street, Leslie Joseph

PA Merck Sharp & Dohme Limited, UK

SO PCT Int. Appl., 46 pp.

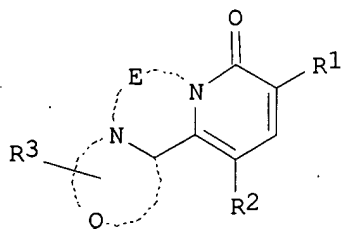
CODEN: PIXXD2

DT Patent

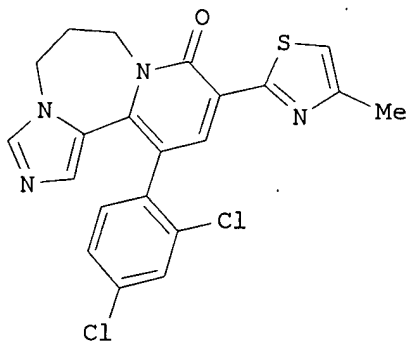
LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|--|----------|-----------------|----------|
| PI | WO 2003018546 | A2 | 20030306 | WO 2002-GB3703 | 20020812 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| PRAI | GB 2001-20345 | A | 20010821 | | |
| OS | MARPAT 138:221605 | | | | |
| GI | | | | | |



I.



II

AB The title fused tricyclic compds. I [$E = (CH_2)_n$; $n = 1-3$; Q = the residue of an imidazole or triazole ring; $R_1, R_2 = H, \text{halo}, \text{heterocyclyl}, \text{etc.}$; $R_3 = H, \text{alkyl}$] which are potent and functionally selective ligands for the α_2/α_3 subunit of the human GABAA receptor and are thereby effective in the treatment of anxiety and convulsions, were prepd. E.g., a 7-step synthesis of II, starting from Et (4-methylthiazol-2-yl)acetate and 3-aminopropanol, was given. The exemplified compds. I were found to possess a K_i of $\text{ltoreq. } 100 \text{ nM}$ for displacement of $[3H]$ -flumazenil from the α_2 and/or α_3 subunit of the human GABAA receptor.

IT 500725-68-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

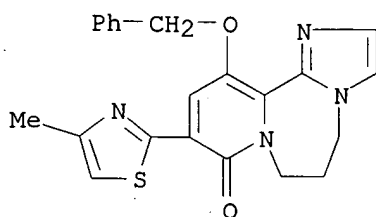
09/868,356

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of tricyclic pyridin-2-one analogs as ligands for GABAA receptors)

RN 500725-68-8 CAPLUS

CN 5H,9H-Imidazo[1,2-a]pyrido[2,1-c][1,4]diazepin-9-one, 6,7-dihydro-10-(4-methyl-2-thiazolyl)-12-(phenylmethoxy)- (9CI) (CA INDEX NAME)



L27 ANSWER 2 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 2002:927175 CAPLUS

DN 138:14131

TI Preparation of pharmaceutical compositions containing mikanolide, dihydromikanolide or an analog thereof combined with another anticancer agent for therapeutic use in cancer treatment

IN Prevost, Gregoire; Coulomb, Helene; Lavergne, Olivier; Lanco, Christophe; Teng, Beng-Poon

PA Societe De Conseils De Recherches Et D'applications Scientifiques (S.C.R.A.S.), Fr.

SO PCT Int. Appl., 103 pp.

CODEN: PIXXD2

DT Patent

LA French

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2002096348 | A2 | 20021205 | WO 2002-FR1800 | 20020529 |
| | W: | | | | |
| | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: | | | | |
| | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | FR 2825278 | A1 | 20021206 | FR 2001-7104 | 20010530 |
| PRAI | FR 2001-7104 | A | 20010530 | | |
| OS | MARPAT 138:14131 | | | | |
| GI | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention concerns a product comprising at least mikanolide (I), dihydromikanolide or an analog, e.g., II [R1 = H, SR4, NR4R5; R2 = SR6, NR6R7; R3 = OH, O-acyl, O-silyl, O-carbamyl; R4, R6 = alkyl, cycloalkyl, (cycloalkyl)alkyl, hydroxyalkyl, (un)substituted aryl, aralkyl; R5, R7 = H, alkyl, cycloalkyl, (cycloalkyl)alkyl, hydroxyalkyl, (un)substituted aryl, aralkyl; R4R5 = 5- to 7-membered N-contg. ring] and III, or their pharmaceutically acceptable salts, combined with at least one other anticancer agent for simultaneous, sep. or prolonged therapeutic use in cancer treatment. In a preferred embodiment of the invention, the mikanolide, dihydromikanolide or one analog thereof is combined with enzymic inhibitors such as G heterotrimeric protein inhibitors, IV [X = R22; Y = R18; XY = 6-membered ring, CHR18CHR19; R11 = H, lower alkyl, alkylthio; R12, R13 = H, lower alkyl; R14 = O, H2; R5 = H, lower alkyl, (cycloalkyl)alkyl, alkenyl, alkynyl, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl; R16, R17 = H, CONHCHR13CO2R14, lower alkyl, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl; R18, R19 = H, lower alkyl, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl; R18R19 = aryl or heterocyclyl ring; R20, R21 = H, aryl, heterocyclyl, alkyl, arylalkyl, heterocyclylalkyl; R22 = NR9, S, O; R23 = ; R24 = H, lower alkyl], V (R18, R19 = H, lower alkyl, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl;

R18R19 = aryl or heterocyclic ring) or VI (R22 = NR9, S, O), or alkylating agents such as cis-platin. Thus, VII was prepd. from mikanolide. VII was tested for cell proliferation inhibition activity [only 34% of cells lived when combined with VIII.cntdot.HCl (vs. human colon cancer HT-29 cells)].

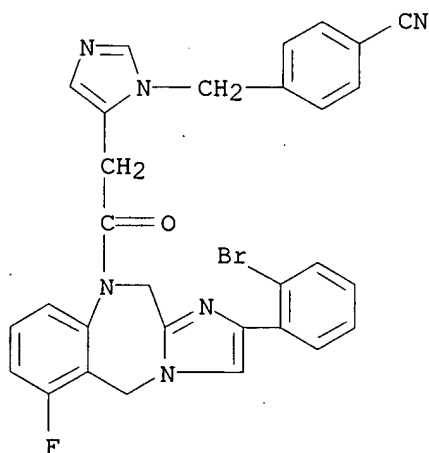
IT **280775-27-1**

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antitumor agent; prepn. of compns. contg. mikanolide, dihydromikanolide or an analog combined with another anticancer agent for chemotherapy)

RN 280775-27-1 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 2-(2-bromophenyl)-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



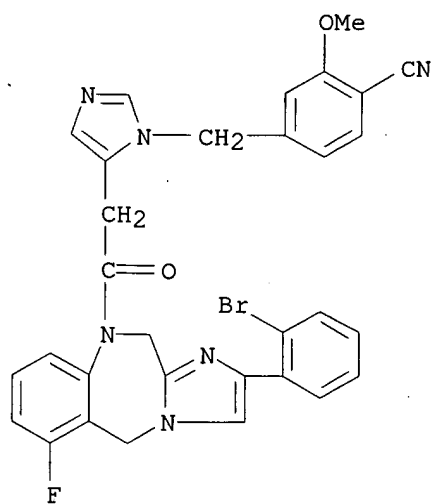
IT **280775-32-8**

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(prepn. of compns. contg. mikanolide, dihydromikanolide or an analog combined with another anticancer agent for chemotherapy)

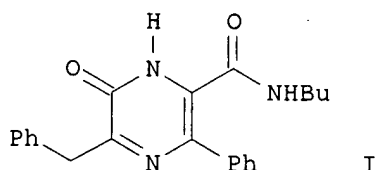
RN 280775-32-8 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 2-(2-bromophenyl)-10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



~~127~~ ANSWER 3 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 2001:816755 CAPLUS
 DN 135:357953
 TI A novel solid support template for preparation of highly functionalized heterocyclic compounds
 IN Campian, Eugene; Lou, Boliang; Yang, Kexin; Zhang, Jinfang
 PA Advanced Syntech, LLC, USA
 SO PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2001083575 | A1 | 20011108 | WO 2001-US823 | 20010109 |
| | W: AU, BR, CA, CN, JP, KR, MX, NO, NZ, US | | | | |
| | RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR | | | | |
| PRAI | US 2000-201285P | P | 20000502 | | |
| OS | CASREACT 135:357953; MARPAT 135:357953 | | | | |
| GI | | | | | |

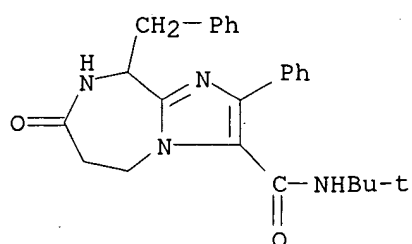


AB R3NHCOCH(COR2)NR4R5 [R = Z2Z1R1; R1 = solid-phase support; R2-R4 = H, alkyl, (hetero)aryl, etc.; R5 = protecting group; Z = (un)substituted CH2, -CH2CH2, -CH:CH, cycloalkylene, etc.; Z1 = multifunctional linker (sic); Z2 = bond or multifunctional chem. monomer possessing .gtoreq.2 attachment points (sic)] were prepd. by Ugi reaction of RNH2, R2COCHO, R3NC, and R4R5NZCO2H and given title use. Thus, deprotected Rink resin was combined with PhCOCHO, BuNC, FMocNHCH(CH2Ph)CO2H, and ZnCl2 to give, in 3 addnl. steps, title compd. I.

IT **371977-53-6P 371977-54-7P**
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (a novel solid support template for prepn. of highly functionalized heterocyclic compds.)

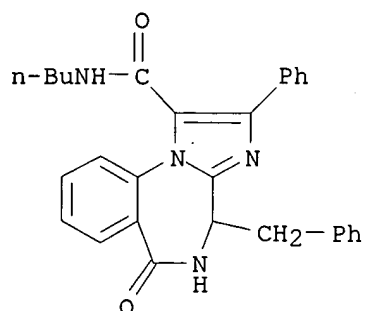
RN 371977-53-6 CAPLUS
 CN 5H-Imidazo[1,2-a][1,4]diazepine-3-carboxamide, N-(1,1-dimethylethyl)-6,7,8,9-tetrahydro-7-oxo-2-phenyl-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

09/868,356



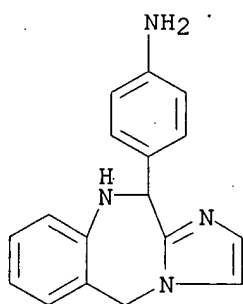
RN 371977-54-7 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-1-carboxamide, N-butyl-5,6-dihydro-6-oxo-2-phenyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



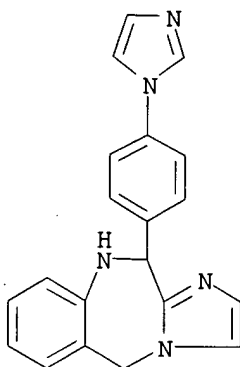
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LN~~ 7 ANSWER 4 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 2001:720352 CAPLUS
 DN 136:193643
 TI Synthesis of 11-aryl-5H-imidazo[2,1-c][1,4]benzodiazepines and their benzodiazepine and A1 adenosine binding activity
 AU Castellano, S.; Zorzin, L.; Florio, C.; Frausin, F.; Stefancich, G.
 CS Dipartimento di Scienze Farmaceutiche, P.le Europa, Trieste, 34127, Italy
 SO Farmaco (2001), 56(10), 771-778
 CODEN: FRMCE8; ISSN: 0014-827X
 PB Elsevier Science S.A.
 DT Journal
 LA English
 AB In the context of a research program aimed at elucidating the properties of the 5H-imidazo[2,1-c][1,4]benzodiazepine system, a series of 11-aryl-5H-imidazo[2,1-c][1,4]benzodiazepines (I) and their 10,11-dihydro derivs. (II) were synthesized. The synthetic strategy includes the prepn. of the aryl-[1-(2-nitrobenzyl)-1H-imidazol-2-yl]methanones followed by their redn. and subsequent cyclization. Affinities of I and II for central benzodiazepine as well as for adenosine A1-receptors were detd. by radioligand binding assays. Among the unsatd. analogs, the highest activity at both receptors is displayed by 11-(2-thienyl) deriv. of I. II did not exhibit considerable binding affinity either for central benzodiazepine or for adenosine A1-receptors.
 IT **401495-55-4P 401495-56-5P 401495-57-6P**
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of 11-aryl-5H-imidazo[2,1-c][1,4]benzodiazepines and benzodiazepine and A1 adenosine binding activity)
 RN 401495-55-4 CAPLUS
 CN Benzenamine, 4-(10,11-dihydro-5H-imidazo[2,1-c][1,4]benzodiazepin-11-yl)-(9CI) (CA INDEX NAME)



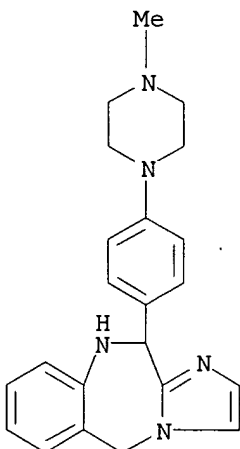
RN 401495-56-5 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-11-[4-(1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)

09/868,356



RN 401495-57-6 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-11-[4-(4-methyl-1-piperazinyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 2001:359845 CAPLUS

DN 134:361346

TI Product inhibiting heterotrimeric G protein signal transduction combined with another anticancer agent for therapeutic use in cancer treatment

IN Prevost, Gregoire; Lonchamp, Marie-Odile; Gordon, Thomas; Morgan, Barry

PA Societe de Conseils de Recherches et d'Applications Scientifiques (S.C.R.A.S.), Fr.

SO PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DT Patent

LA French

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2001034203 | A1 | 20010517 | WO 2000-FR3098 | 20001108 |
| | W: | | | | |
| | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: | | | | |
| | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | FR 2800616 | A1 | 20010511 | FR 1999-14037 | 19991109 |
| | FR 2800616 | B1 | 20020118 | | |
| | FR 2803524 | A1 | 20010713 | FR 2000-104 | 20000106 |
| | FR 2803524 | B1 | 20020419 | | |
| | EP 1233787 | A1 | 20020828 | EP 2000-976116 | 20001108 |
| | R: | | | | |
| | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| PRAI | FR 1999-14037 | A | 19991109 | | |
| | FR 2000-104 | A | 20000106 | | |
| | WO 2000-FR3098 | W | 20001108 | | |

OS MARPAT 134:361346

AB The invention provides a product inhibiting heterotrimeric G protein signal transduction combined with another anticancer agent, in particular a farnesyltransferase inhibitor, taxol or gemcitabine, for simultaneous, sep., or prolonged therapeutic use in cancer treatment.

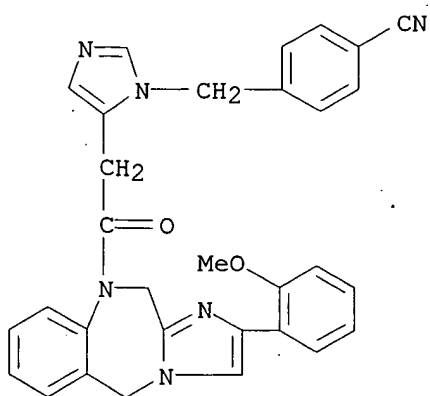
IT 280775-15-7 280775-32-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(heterotrimeric G protein signal transduction inhibitor combined with another anticancer agent for cancer treatment)

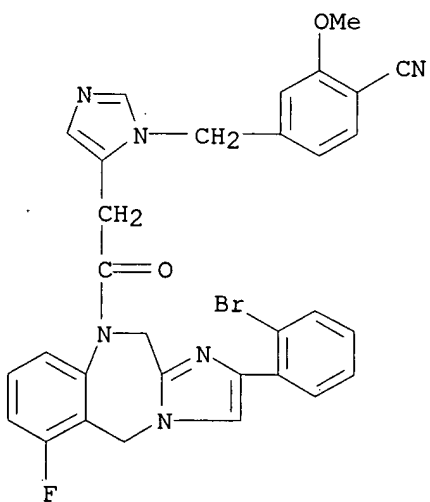
RN 280775-15-7 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



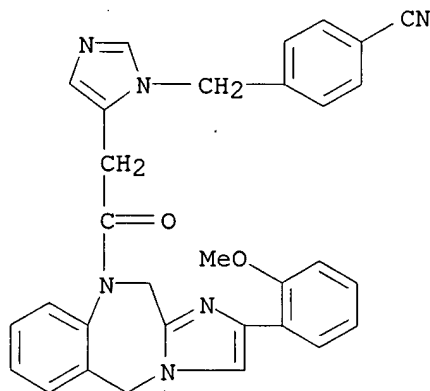
RN 280775-32-8 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 2-(2-bromophenyl)-10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

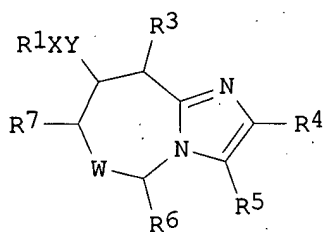
~~DOI~~ ANSWER 6 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 2001:128354 CAPLUS
 DN 135:174767
 TI Inhibition of human tumor cell growth in vivo by an orally bioavailable inhibitor of human farnesyltransferase, BIM-46228
 AU Prevost, Gregoire P.; Pradines, Anne; Brezak, Marie-Christine; Lonchampt, Marie-Odile; Viossat, Isabelle; Ader, Isabelle; Toulas, Christine; Kasprzyk, Philip; Gordon, Thomas; Favre, Gilles; Morgan, Barry
 CS Institut Henri Beaufour, Les Ulis, F-91966, Fr.
 SO International Journal of Cancer (2001), 91(5), 718-722
 CODEN: IJCNAA; ISSN: 0020-7136
 PB Wiley-Liss, Inc.
 DT Journal
 LA English
 AB This work reports a novel farnesyltransferase inhibitor, BIM-46228, which gave: (1) specific inhibition of purified human farnesyltransferase enzyme, (2) inhibition of proliferation of a broad spectrum of human tumor cell lines in vitro, (3) inhibition of the growth of human tumor xenografts in athymic nude mice treated orally and (4) combination of its activity with chemotherapy (paclitaxel) or radiotherapy in vitro.
 IT **280775-15-7, BIM 46228**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (inhibition of human tumor cell growth by an orally bioavailable inhibitor of human farnesyltransferase, BIM-46228)
 RN 280775-15-7 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 7 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 2000:457071 CAPLUS
 DN 133:89553
 TI Preparation of imidazopyrazines, imidazobenzodiazepines, and related compounds as prenyl transferase inhibitors.
 IN Gordon, Thomas B.; Morgan, Barry A.
 PA Societe de Conseils de Recherches et d'Applications Scientifiques S.A., Fr.
 SO PCT Int. Appl., 95 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|------------------|--|----------|-----------------|----------|
| PI | WO 2000039130 | A2 | 20000706 | WO 1999-US31302 | 19991230 |
| | WO 2000039130 | A3 | 20001102 | | |
| | W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | CA 2356756 | AA | 20000706 | CA 1999-2356756 | 19991230 |
| | EP 1140942 | A2 | 20011010 | EP 1999-968984 | 19991230 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | |
| | NO 2001003281 | A | 20010829 | NO 2001-3281 | 20010629 |
| PRAI | US 1998-114301P | P | 19981231 | | |
| | US 1998-224428 | A1 | 19981231 | | |
| | WO 1999-US31302 | W | 19991230 | | |
| OS | MARPAT 133:89553 | | | | |
| GI | | | | | |



AB Title compds. [I; X = (CHR11)n3(CH2)n4Z(CH2)n5; n3 = 0, 1; n4, n5 = 0-3; Z = O, NR12, S, bond; Y = CO, CH2, CS, bond; R1 = (substituted) imidazolyl, triazolyl, tetrazolyl, benzimidazolyl, isoquinolinyl, pyridyl, etc.; R3 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, cycloalkenyl, cycloalkenylalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; R4, R5 = H, (substituted) alkyl, cycloalkyl, aryl, heterocyclyl; R6 = H, (substituted) alkyl, alkenyl, cycloalkyl,

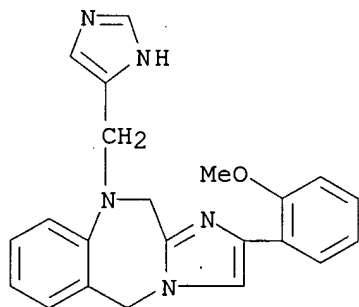
cycloalkylalkyl, cycloalkenyl, cycloalkenylalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; R7 = H, :O, :S, (substituted) alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, cycloalkenyl, cycloalkenylalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; W = null, C], were prepd. as prenyl transferase inhibitors (no data). Thus, 1-(2-ethoxy-2-oxoethyl)-2-[(1S)-[(phenylmethoxy)carbonyl]amino]pentyl]-4-(2-methoxyphenyl)imidazole (prepn. given) was hydrogenated in HOAc over Pd/C to give 8-butyl-6-oxo-2-(2-methoxyphenyl)imidazo[1,2-a]pyrazine. This was converted to 8-butyl-7-[3-(imidazol-5-yl)-1-oxopropyl]-2-(2-methoxyphenyl)-5,6,7,8-tetrahydroimidazo[1,2-a]pyrazine in several steps.

IT 280775-14-6P 280775-15-7P 280775-16-8P
 280775-17-9P 280775-18-0P 280775-19-1P
 280775-21-5P 280775-22-6P 280775-23-7P
 280775-24-8P 280775-25-9P 280775-26-0P
 280775-27-1P 280775-28-2P 280775-29-3P
 280775-30-6P 280775-31-7P 280775-32-8P
 280775-33-9P 280775-34-0P 280775-65-7P
 280775-68-0P 280775-69-1P 280775-70-4P
 280775-71-5P 280775-72-6P 280775-73-7P
 280775-82-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of imidazopyrazines, imidazobenzodiazepines, and related compds. as prenyl transferase inhibitors)

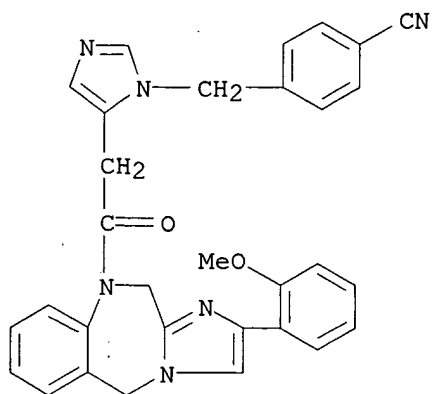
RN 280775-14-6 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-10-(1H-imidazol-4-ylmethyl)-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



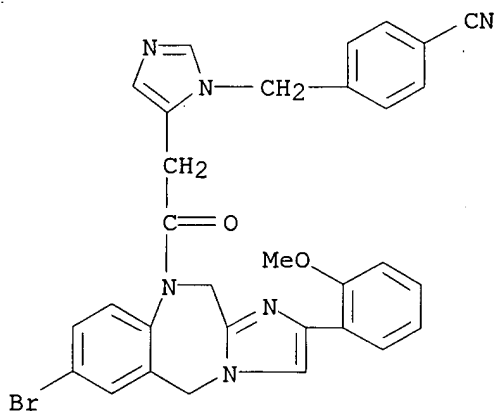
RN 280775-15-7 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



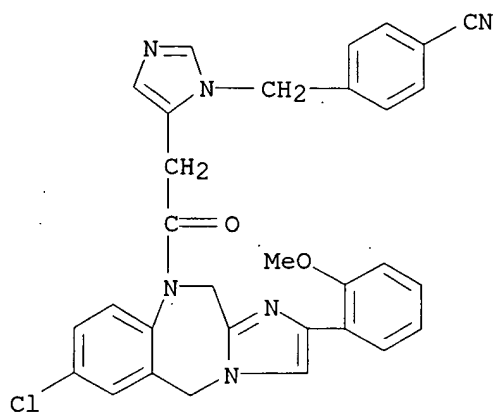
RN 280775-16-8 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 7-bromo-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



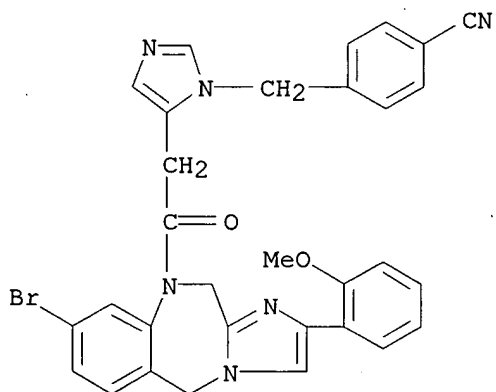
RN 280775-17-9 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 7-chloro-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



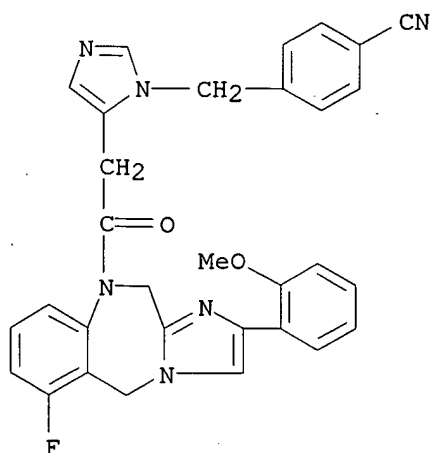
RN 280775-18-0 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 8-bromo-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



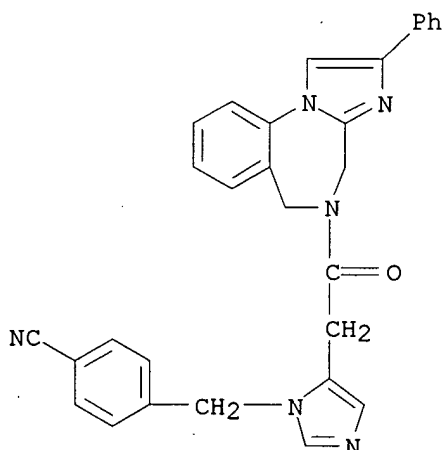
RN 280775-19-1 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



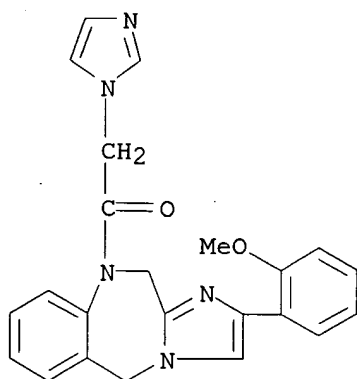
RN 280775-21-5 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine, 5-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-5,6-dihydro-2-phenyl- (9CI) (CA INDEX NAME)



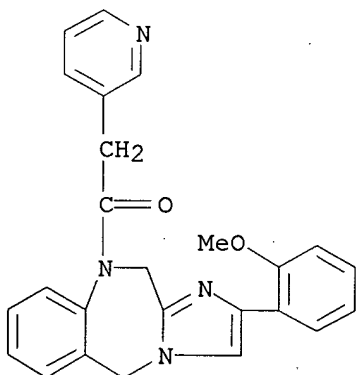
RN 280775-22-6 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-10-(1H-imidazol-1-ylacetyl)-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



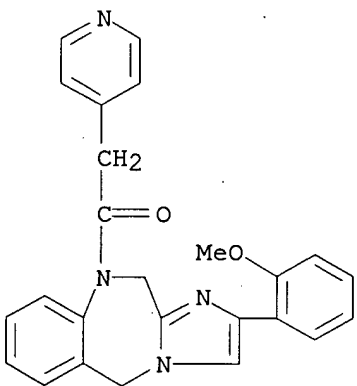
RN 280775-23-7 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-2-(2-methoxyphenyl)-10-(3-pyridinylacetyl)- (9CI) (CA INDEX NAME)



RN 280775-24-8 CAPLUS

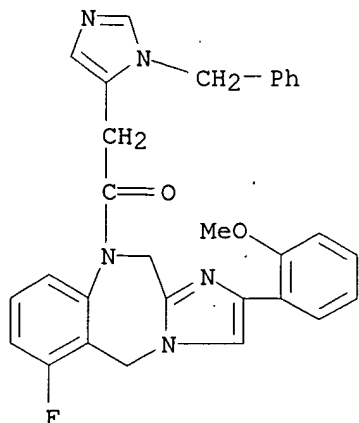
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-2-(2-methoxyphenyl)-10-(4-pyridinylacetyl)- (9CI) (CA INDEX NAME)



RN 280775-25-9 CAPLUS

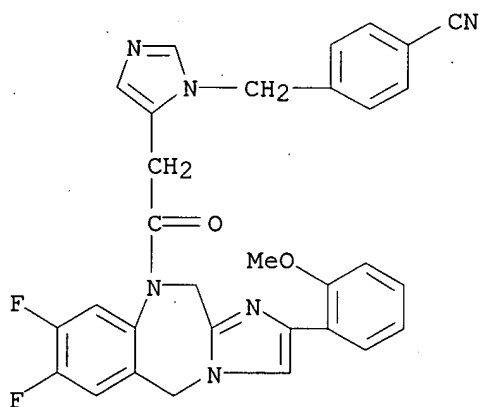
09/868,356

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)-10-[[1-(phenylmethyl)-1H-imidazol-5-yl]acetyl]- (9CI) (CA INDEX NAME)



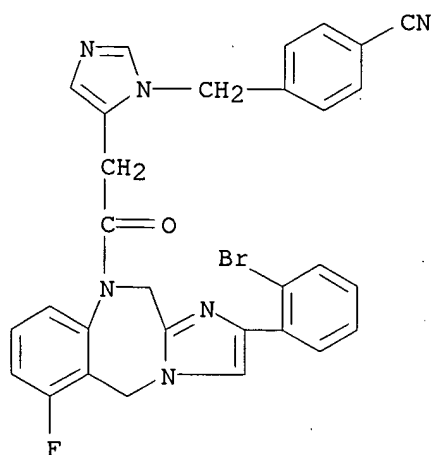
RN 280775-26-0 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-7,8-difluoro-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



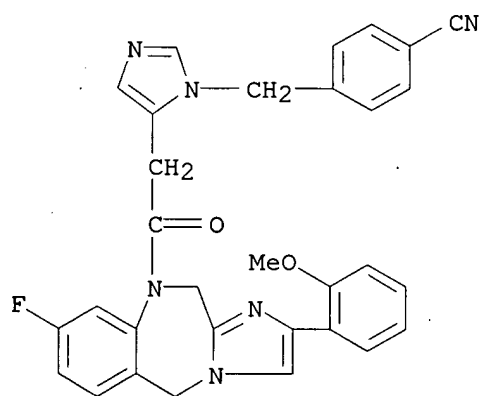
RN 280775-27-1 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 2-(2-bromophenyl)-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



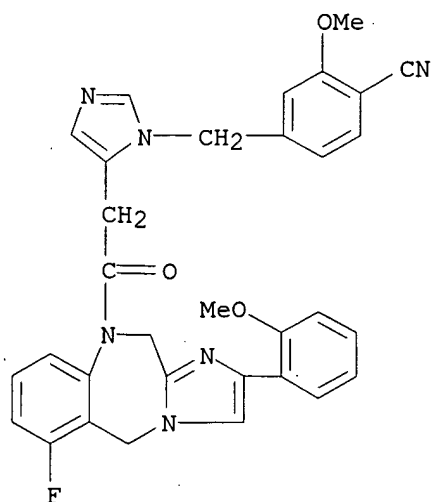
RN 280775-28-2 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-8-fluoro-10,11-dihydro-2-(2-methoxyphenyl)- (9CI)
(CA INDEX NAME)



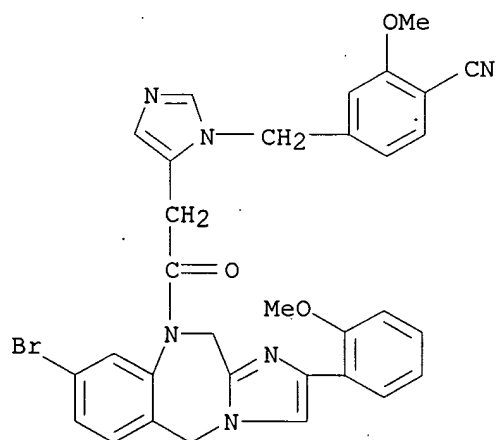
RN 280775-29-3 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



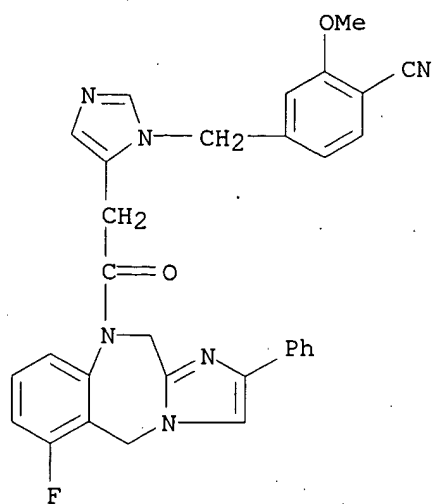
RN 280775-30-6 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 8-bromo-10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



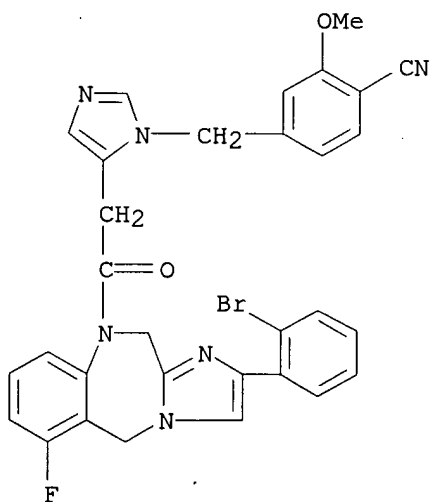
RN 280775-31-7 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro-2-phenyl- (9CI) (CA INDEX NAME)



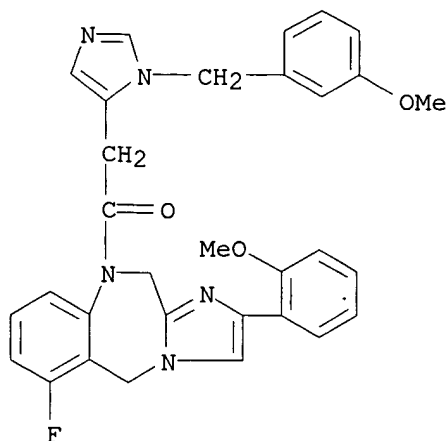
RN 280775-32-8 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 2-(2-bromophenyl)-10-[[1-[(4-cyano-3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro-
(9CI) (CA INDEX NAME)



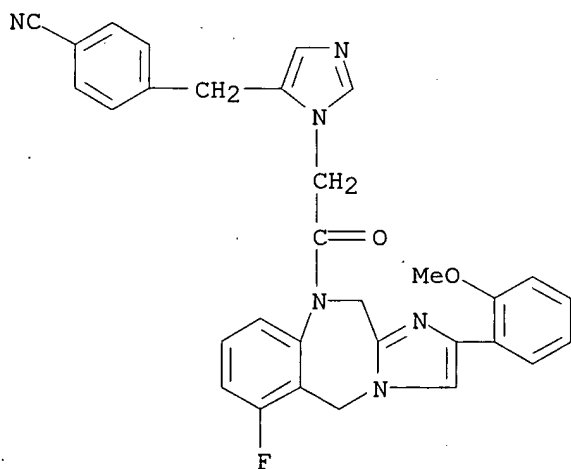
RN 280775-33-9 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)-10-[[1-[(3-methoxyphenyl)methyl]-1H-imidazol-5-yl]acetyl]-
(9CI) (CA INDEX NAME)



RN 280775-34-0 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[5-[(4-cyanophenyl)methyl]-1H-imidazol-1-yl]acetyl]-6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)- (9CI)
(CA INDEX NAME)



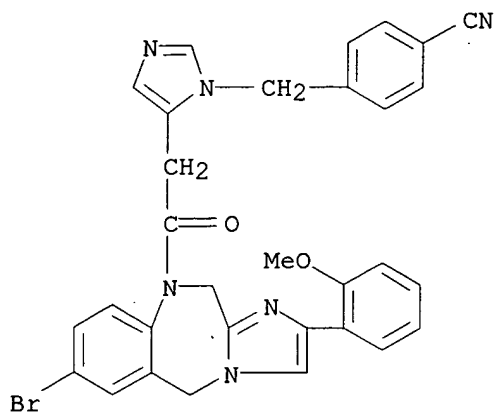
RN 280775-65-7 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 7-bromo-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 280775-16-8

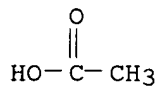
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CM 2

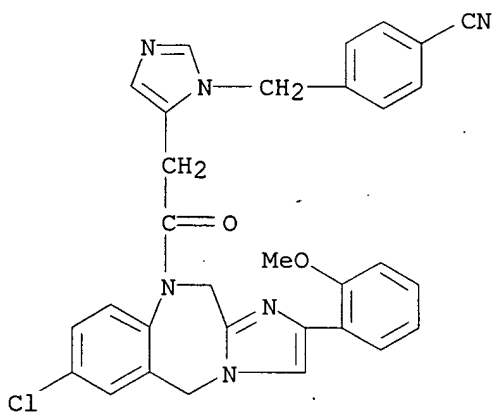
CRN 64-19-7

CMF C2 H4 O2



RN 280775-68-0 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 7-chloro-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)

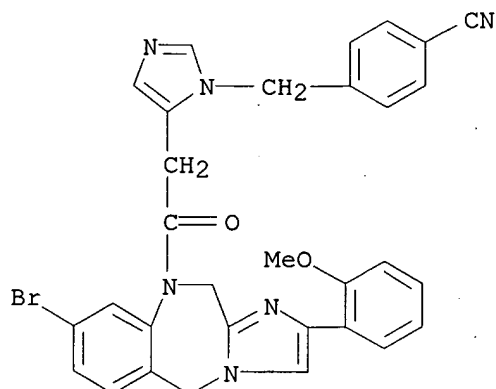


● 2 HCl

RN 280775-69-1 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 8-bromo-10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-

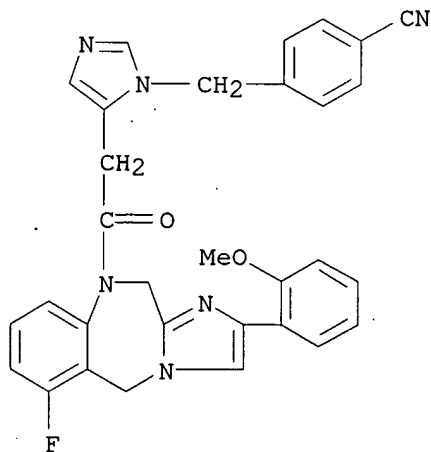
methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 280775-70-4 CAPLUS

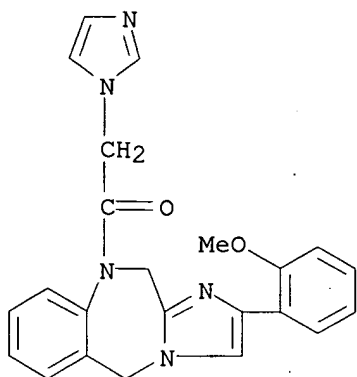
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

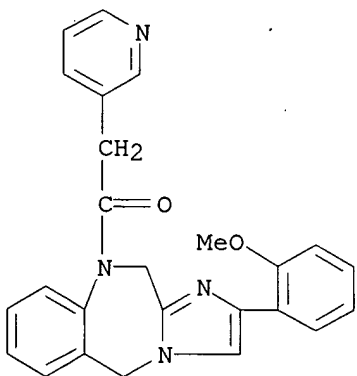
RN 280775-71-5 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-10-(1H-imidazol-1-ylacetyl)-2-(2-methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



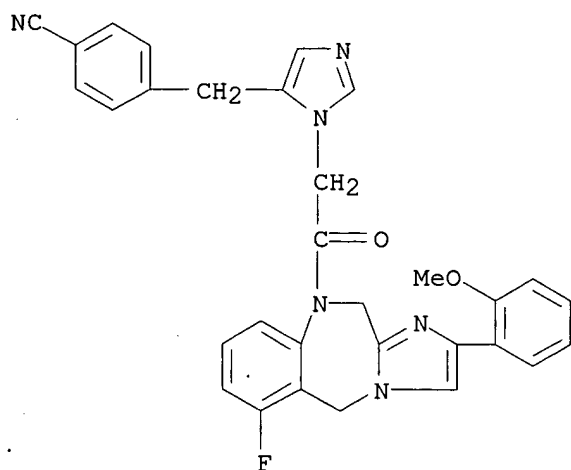
●2 HCl

RN 280775-72-6 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-2-(2-methoxyphenyl)-10-(3-pyridinylacetyl)-, dihydrochloride (9CI) (CA INDEX NAME)



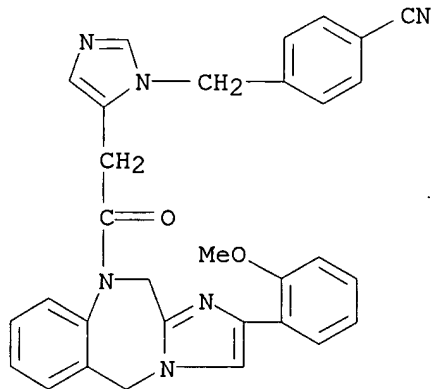
●2 HCl

RN 280775-73-7 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[5-[(4-cyanophenyl)methyl]-1H-imidazol-1-yl]acetyl]-6-fluoro-10,11-dihydro-2-(2-methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



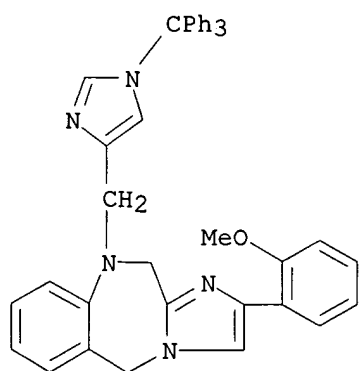
●2 HCl

RN 280775-82-8 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-[[1-[(4-cyanophenyl)methyl]-1H-imidazol-5-yl]acetyl]-10,11-dihydro-2-(2-methoxyphenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



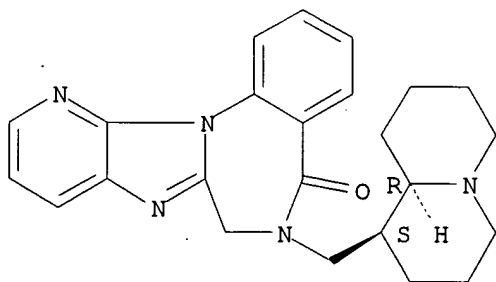
●2 HCl

IT **280775-63-5P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of imidazopyrazines, imidazobenzodiazepines, and related compds. as prenyl transferase inhibitors)
 RN 280775-63-5 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-2-(2-methoxyphenyl)-10-[[1-(triphenylmethyl)-1H-imidazol-4-yl]methyl]- (9CI) (CA INDEX NAME)



~~120~~ ANSWER 8 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1999:716689 CAPLUS
 DN 132:73216
 TI Quinolizidinyl derivatives of 5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one as ligands for muscarinic receptors
 AU Novelli, Federica; Sparatore, Anna; Tasso, Bruno; Sparatore, Fabio
 CS Dipartimento di Scienze Farmaceutiche - Universita di Genova, Genoa, 3 - 16132, Italy
 SO Bioorganic & Medicinal Chemistry Letters (1999), 9(20), 3031-3034
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 AB Quinolizidinyl derivs. of the tricyclic systems characterizing pirenzepine and nuvenzepine, were prepd. and tested as ligands for muscarinic M1, M2 and M3 receptors; 5,11-dihydro-11-[(S-lupinyl)-thioacetyl]-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one exhibited IC50 = 10 nM for M1 and 760 nM for both M2 and M3 subtypes. A compd. bearing quinolizidine nucleus linked equatorially exhibited higher affinity to muscarinic receptors than its axial epimer. During the synthesis some interesting side compds. were isolated and characterized.
 IT **253609-42-6P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)
 (quinolizidinyl derivs. of pyridobenzodiazepine as ligands for muscarinic receptors)
 RN 253609-42-6 CAPLUS
 CN 5H-Pyrido[3',2':4,5]imidazo[1,2-a][1,4]benzodiazepin-5-one, 6,7-dihydro-6-[[(1R,9aS)-octahydro-2H-quinolizin-1-yl]methyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/868,356

~~127~~ ANSWER 9 OF 46 CAPLUS COPYRIGHT 2003 ACS

~~IN~~ 1999:38608 CAPLUS

~~DN~~ 130:182376

TI Preparation and biological activity of novel tricyclic GPIIb/IIIa antagonists

AU Robargè, Kirk D.; Dina, Michael S.; Somers, Todd C.; Lee, Arthur; Rawson, Thomas E.; Olivero, Alan G.; Tischler, Maureen H.; Webb, Robert R., II; Weese, Kenneth J.; Aliagas, Ignacio; Blackburn, Brent K.

CS Department of Bioorganic Chemistry, Genentech, Inc., South San Francisco, CA, 94080, USA

SO Bioorganic & Medicinal Chemistry (1998), 6(12), 2345-2381

CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

AB Antagonists of the glycoprotein GPIIb/IIIa are a promising class of antithrombotic agents offering potential advantages over present antiplatelet agents (i.e., aspirin and ticlopidine). Novel tricyclic nonpeptidic GPIIb/IIIa antagonists have been prepared and evaluated in vitro as antagonists of fibrinogen binding to the purified GPIIb/IIIa receptor and as inhibitors of platelet aggregation. The work presented demonstrates the robustness of the benzodiazepinedione (BZDD) scaffold, which can be functionalized at the N1-C2 amide as well as at C7, to provide structural diversity and allow optimization of the physiochem. and pharmacol. properties of the BZDD based GPIIb/IIIa antagonists. In addition, the resulting new class of tricyclic GPIIb/IIIa antagonists could be used to probe for additional binding interactions on the GPIIb/IIIa receptor and perhaps lead to BZDD based GPIIb/IIIa antagonists with increased potency.

IT 167853-81-8P 167855-32-5P 167855-44-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of tricyclic GPIIb/IIIa antagonists)

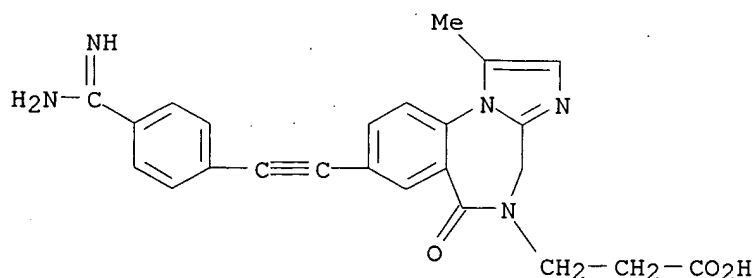
RN 167853-81-8 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167853-80-7

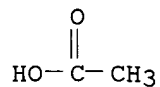
CMF C24 H21 N5 O3



CM 2

09/868,356

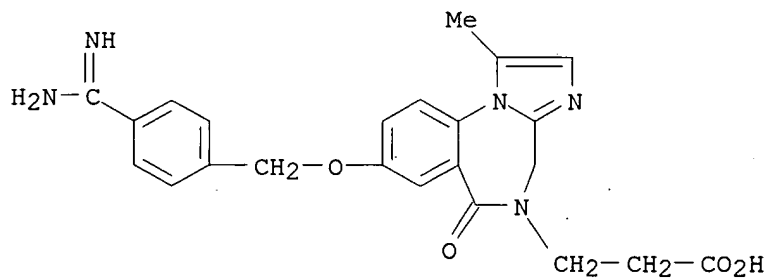
CRN 64-19-7
CMF C2 H4 O2



RN 167855-32-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]methoxy]-1-methyl-6-oxo-, monoacetate (9CI)
(CA INDEX NAME)

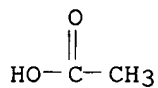
CM 1

CRN 167855-31-4
CMF C23 H23 N5 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

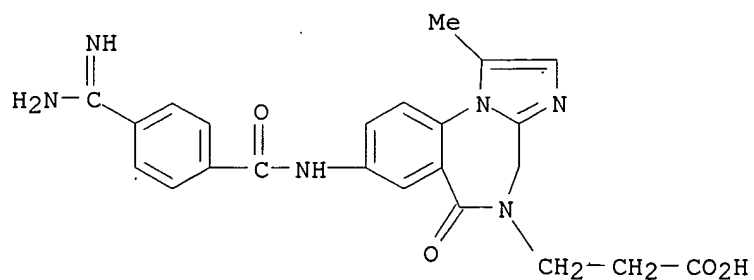


RN 167855-44-9 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167855-43-8
CMF C23 H22 N6 O4

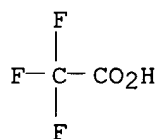
09/868,356



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 167853-92-1P 167853-94-3P 167853-95-4P

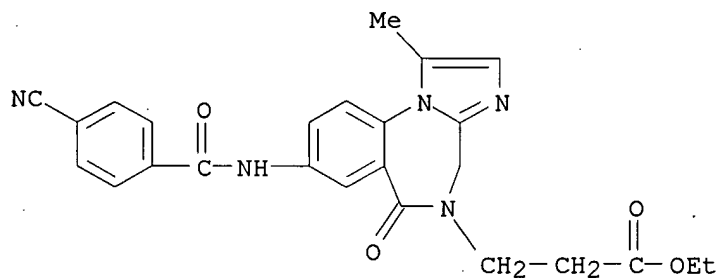
167854-00-4P 167854-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of tricyclic GPIIb/IIIa antagonists)

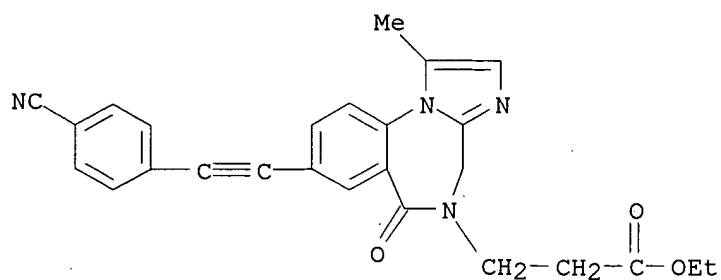
RN 167853-92-1 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[(4-cyanobenzoyl)amino]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)

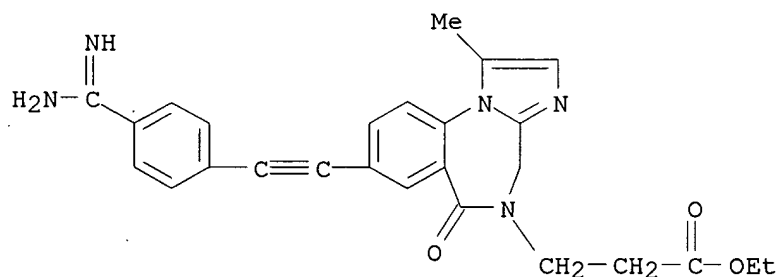


RN 167853-94-3 CAPLUS

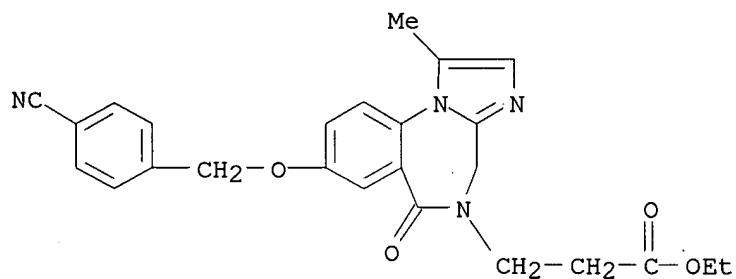
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[(4-cyanophenyl)ethynyl]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 167853-95-4 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, ethyl ester (9CI)
 (CA INDEX NAME)

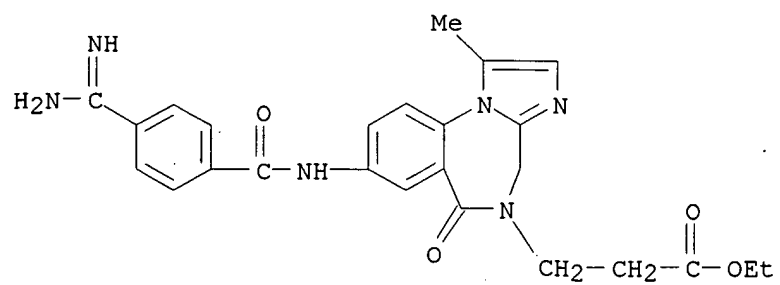


RN 167854-00-4 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(4-cyanophenyl)methoxy]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
 NAME)



RN 167854-15-1 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(4-aminophenyl)benzoyl]amino]-1-methyl-6-oxo-, ethyl ester (9CI)
 (CA INDEX NAME)

09/868,356



RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~127~~ ANSWER 10 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1998:479505 CAPLUS

DN 129:122870

TI Preparation of cycloalkyl, lactam, lactone and related compounds for inhibiting .beta.-amyloid peptide release and/or its synthesis

IN Wu, Jing; Tung, Jay S.; Thorsett, Eugene D.; Pleiss, Michael A.; Nissen, Jeffrey S.; Neitz, Jeffrey; Latimer, Lee H.; John, Varghese; Freedman, Stephen; Britton, Thomas C.; Audia, James E.; Reel, Jon K.; Mabry, Thomas E.; Dressman, Bruce A.; Cwi, Cynthia L.; Droste, James J.; Henry, Steven S.; Mcdaniel, Stacey L.; Scott, William Leonard; Stucky, Russell D.; Porter, Warren J.

PA Athena Neurosciences, Inc., USA; Eli Lilly & Co.

SO PCT Int. Appl., 889 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|--|----------|-----------------|----------|
| PI | WO 9828268 | A2 | 19980702 | WO 1997-US22986 | 19971222 |
| | WO 9828268 | A3 | 19981008 | | |
| | W: | AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | |
| | ZA 9711537 | A | 19980625 | ZA 1997-11537 | 19971222 |
| | AU 9857007 | A1 | 19980717 | AU 1998-57007 | 19971222 |
| | AU 749658 | B2 | 20020627 | | |
| | EP 951466 | A2 | 19991027 | EP 1997-953208 | 19971222 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | |
| | CN 1242007 | A | 20000119 | CN 1997-180901 | 19971222 |
| | BR 9714517 | A | 20000704 | BR 1997-14517 | 19971222 |
| | JP 2000511932 | T2 | 20000912 | JP 1998-528867 | 19971222 |
| | NZ 335583 | A | 20010330 | NZ 1997-335583 | 19971222 |
| | MX 9905844 | A | 20000731 | MX 1999-5844 | 19990621 |
| | NO 9903098 | A | 19990820 | NO 1999-3098 | 19990622 |
| | US 2002045747 | A1 | 20020418 | US 2001-916282 | 20010730 |
| | US 2002055500 | A1 | 20020509 | US 2001-916440 | 20010730 |
| PRAI | US 1996-64851P | P | 19961223 | | |
| | US 1996-64851P | P | 19961223 | | |
| | US 1996-780025 | A1 | 19961223 | | |
| | US 1997-996422 | A3 | 19971222 | | |
| | WO 1997-US22986 | W | 19971222 | | |
| OS | MARPAT 129:122870 | | | | |
| AB | Disclosed are compds. R1ZmNHYNCHpR2C(X)R3 [R1 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, or cycloalkenyl or aryl, heteroaryl, or heterocyclic; R2 and R3 form a cycloalkyl, cycloalkenyl, heterocyclic, substituted cycloalkyl, or substituted cycloalkenyl ring which is optionally fused; X = oxo, thioxo, hydroxyl, thiol, or hydro; Y = CHR4CONH where R4 = (un)substituted alkyl, alkenyl, or alkynyl or cycloalkyl, aryl, heteroaryl, or heterocyclic; Z is TCX'X''CO where T is a bond, O, S, NR5 (R5 = H, acyl, alkyl, aryl, or heteroaryl), X' and X'' are H, OH, or F or X'X'' = oxo; m, p = 0, 1; n = 0, 1, 2] which inhibit .beta.-amyloid | | | | |

peptide release and/or its synthesis, and, accordingly, have utility in treating Alzheimer's disease. Thus, 3-[[N'-(3,4-methylenedioxyphenylacetyl)-L-alaninyl]amino]-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepin-2-one was prepd. by coupling of 3-(L-alaninylamino)-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepin-2-one with 3,4-methylenedioxyphenylacetic acid.

IT **209996-34-9P**

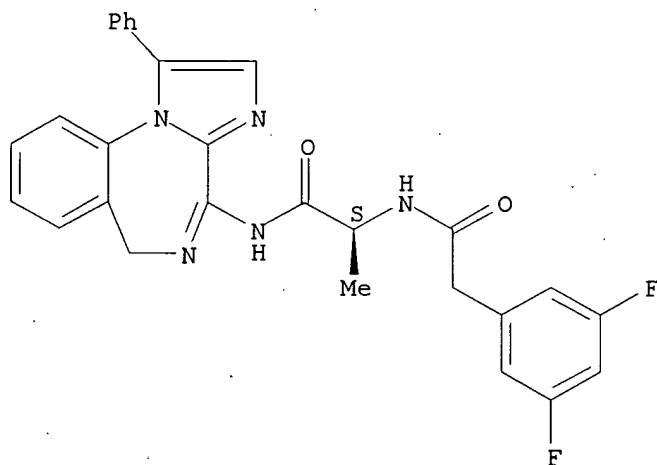
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of cycloalkyl, lactam, lactone and related compds. for inhibiting .beta.-amyloid peptide release and/or its synthesis)

RN 209996-34-9 CAPLUS

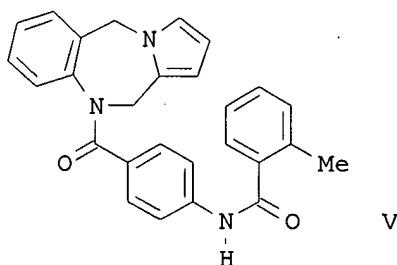
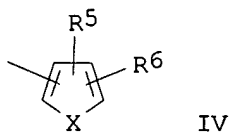
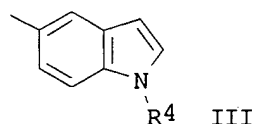
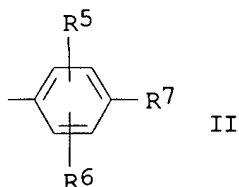
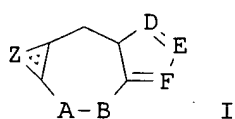
CN Benzeneacetamide, 3,5-difluoro-N-[(1S)-1-methyl-2-oxo-2-[(1-phenyl-6H-imidazo[1,2-a][1,4]benzodiazepin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



~~127~~ ANSWER 11 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1998:219348 CAPLUS
 DN 128:282852
 TI Tricyclic diazepine vasopressin and oxytocin antagonists
 IN Albright, Jay Donald; Reich, Marvin Fred; Sum, Fuk-Wah; Santos, Efren
 Guillermo Delos
 PA American Cyanamid Company, USA
 SO U.S., 132 pp., Cont.-in-part of U.S. 5,624,923.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|------|----------|-----------------|----------|
| PI | US 5736540 | A | 19980407 | US 1996-646841 | 19960508 |
| | US 5516774 | A | 19960514 | US 1994-254822 | 19940613 |
| | US 5624923 | A | 19970429 | US 1995-468737 | 19950606 |
| PRAI | US 1993-100004 | B2 | 19930729 | | |
| | US 1994-254822 | A3 | 19940613 | | |
| | US 1995-468737 | A2 | 19950606 | | |
| OS | MARPAT 128:282852 | | | | |
| GI | | | | | |



AB Title compds. [I; A-B = (CH₂)NR₃ or NR₃CH₂; D, E, F = (un)substituted C or N; Z = atoms to complete an (un)substituted (hetero)arom. ring; R₃ = COAr, wherein Ar is selected from (hetero)aryl groups II-IV; X = O, S, NH, NMe, NAc; R₄ = H, lower alkyl, etc.; R₅ = H, lower alkyl, etc.; R₆ = amido, aminocarbonyl, ureido, etc.; R₇ = H, lower alkyl, etc.] were prepd. Thus, amidation of 4-[(2-methylbenzoyl)amino]benzoyl chloride with 10,11-dihydro-5H-pyrrolo[2,1-c][1,4]benzodiazepine afforded benzamide V which at 1-10 mg/kg exhibited vasopressin V₂ antagonist activity in conscious hydrated rats (increased urine vol. and decreased osmolality relative to control), vasopressin V₁ antagonist activity (e.g., 70% inhibition of vasopressin vasopressor response in conscious rats at 3

mg/kg i.v.), and 90% inhibition of oxytocin receptor binding at 10 μ M with $IC_{50} = 0.36 \mu$ M. V exhibited binding to rat hepatic V1 receptors and rat kidney medullary V2 receptors with $IC_{50} = 0.038$ and 0.004μ M, resp.

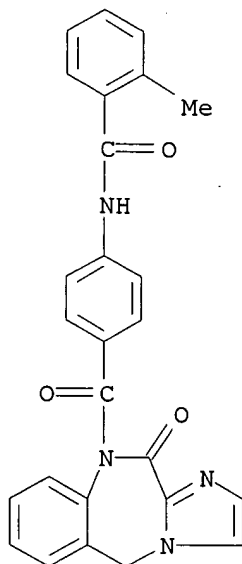
IT 179063-03-7P 179063-04-8P 179063-05-9P

179063-06-0P 179063-10-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tricyclic diazepine vasopressin antagonists and oxytocin antagonists)

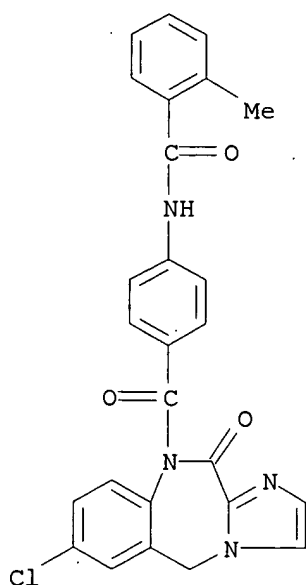
RN 179063-03-7 CAPLUS

CN Benzamide, 2-methyl-N-[4-[(11-oxo-5H-imidazo[2,1-a][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



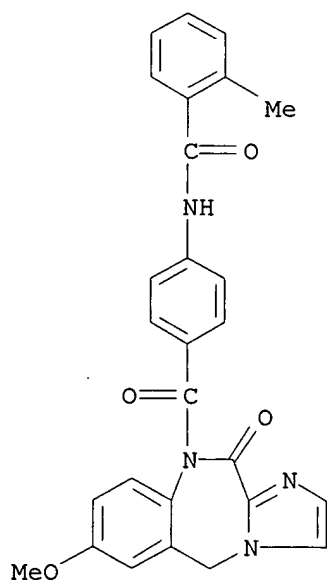
RN 179063-04-8 CAPLUS

CN Benzamide, N-[4-[(7-chloro-11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



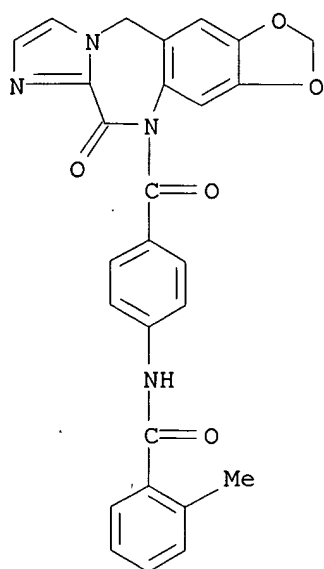
RN 179063-05-9 CAPLUS

CN Benzamide, N-[4-[(7-methoxy-11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)

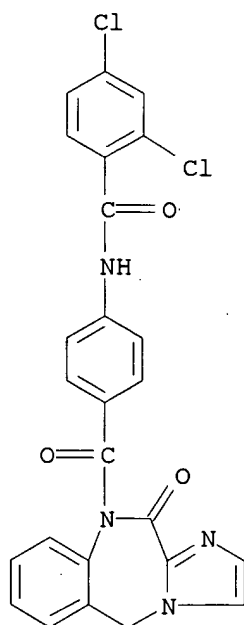


RN 179063-06-0 CAPLUS

CN Benzamide, 2-methyl-N-[4-[(6-oxo-6H-1,3-dioxolo[4,5-h]imidazo[2,1-c][1,4]benzodiazepin-5(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



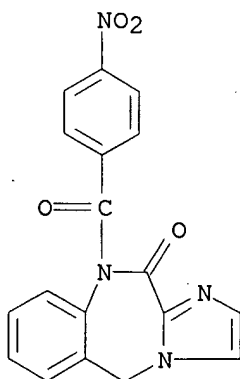
RN 179063-10-6 CAPLUS
 CN Benzamide, 2,4-dichloro-N-[4-[(11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



IT 179063-15-1P 179063-16-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (tricyclic diazepine vasopressin antagonists and oxytocin antagonists)
 RN 179063-15-1 CAPLUS
 CN 11H-Imidazo[2,1-c][1,4]benzodiazepin-11-one, 5,10-dihydro-10-(4-

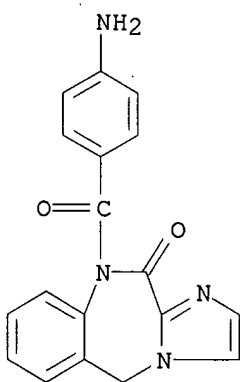
09/868,356

nitrobenzoyl)- (9CI) (CA INDEX NAME)



RN 179063-16-2 CAPLUS

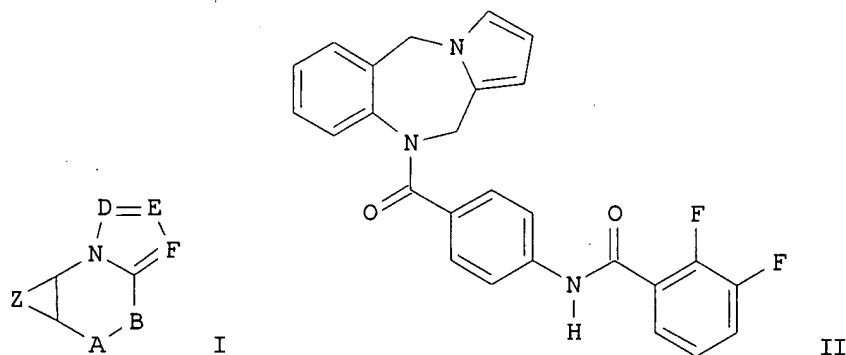
CN 11H-Imidazo[2,1-c][1,4]benzodiazepin-11-one, 10-(4-aminobenzoyl)-5,10-dihydro- (9CI) (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~127~~ ANSWER 12 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1998:202669 CAPLUS
 DN 128:257452
 TI Preparation of tricyclic diazepine vasopressin antagonists and oxytocin antagonists
 IN Albright, Jay Donald; Reich, Marvin Fred; Sum, Fuk-Wah; Santos, Efren Guillermo Delos
 PA American Cyanamid Company, USA
 SO U.S., 126 pp., Cont.-in-part of U.S. 5,624,923.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|------|----------|-----------------|----------|
| PI | US 5733905 | A | 19980331 | US 1996-646582 | 19960508 |
| | US 5516774 | A | 19960514 | US 1994-254822 | 19940613 |
| | US 5624923 | A | 19970429 | US 1995-468737 | 19950606 |
| | US 5854237 | A | 19981229 | US 1997-877314 | 19970617 |
| | US 5843944 | A | 19981201 | US 1997-893636 | 19970711 |
| PRAI | US 1993-100004 | B2 | 19930729 | | |
| | US 1994-254822 | A3 | 19940613 | | |
| | US 1995-468737 | A2 | 19950606 | | |
| | US 1996-646582 | A1 | 19960508 | | |
| OS | MARPAT 128:257452 | | | | |
| GI | | | | | |



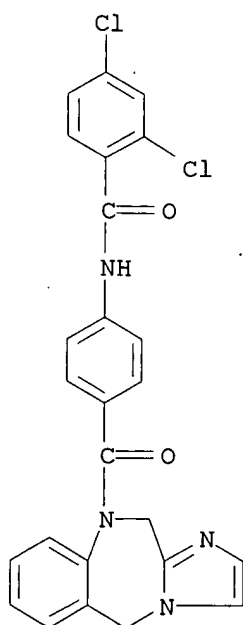
AB The title compds. [I; A-B = N(R₃)(CH₂)₂; fused ring contg. Z = (un)substituted fused phenyl; D, E, F = (un)substituted C, N], which have vasopressin and oxytocin antagonist activity and therefore are useful for treating disease in a mammal characterized by excess renal reabsorption of water such as congestive heart failure, nephrotic syndrome, hyponatremia, coronary vasospasm, cardiac ischemia, liver cirrhosis, brain edema, cerebral ischemia, cerebral hemorrhage-stroke, were prepd. Thus, reaction of 2,3-difluorobenzoyl chloride with 10,11-dihydro-10-(4-aminobenzoyl)-5H-pyrrolo[2.1-c][1,4]benzodiazepine in the presence of Et₃N in CH₂Cl₂ afforded the title compd. II which showed IC₅₀ of 0.097 .mu.M against rat hepatic V1 receptors binding, and IC₅₀ of 0.029 .mu.M against rat kidney medullary V2 receptors binding.

IT 168080-00-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tricyclic diazepine vasopressin antagonists and oxytocin antagonists)

RN 168080-00-0 CAPLUS

CN Benzamide, 2,4-dichloro-N-[4-(5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)



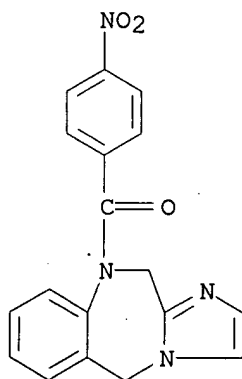
IT 168078-74-8P 168078-75-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of tricyclic diazepine vasopressin antagonists and oxytocin antagonists)

RN 168078-74-8 CAPLUS

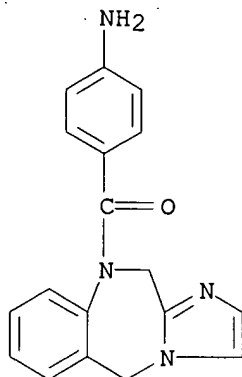
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-10-(4-nitrobenzoyl)- (9CI) (CA INDEX NAME)



09/868,356

RN 168078-75-9 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-(4-aminobenzoyl)-10,11-dihydro-
(9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~127~~ ANSWER 13 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1998:31206 CAPLUS

DN 128:114969

TI Preparation of tricyclic benzodiazepines as inhibitors of the GPIIb/IIIa receptor.

IN Blackburn, Brent K.; Robarge, Kirk; Somers, Todd C.

PA Genentech, Inc., USA

SO U.S., 156 pp., Cont.-in-part of U.S. 5,493,020.

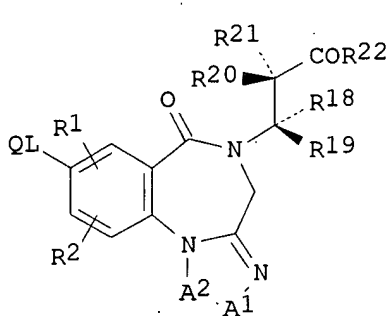
CODEN: USXXAM

DT Patent

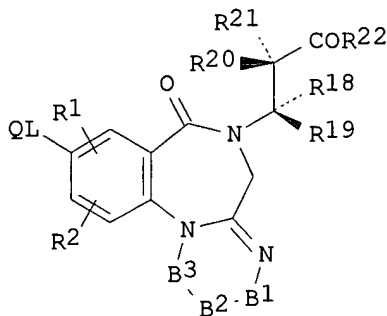
LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | US 5705890 | A | 19980106 | US 1994-313069 | 19940926 |
| | US 5493020 | A | 19960220 | US 1993-99019 | 19930729 |
| | WO 9504057 | A1 | 19950209 | WO 1994-US7989 | 19940715 |
| | W: CA, JP, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | US 5716951 | A | 19980210 | US 1995-438143 | 19950508 |
| PRAI | US 1993-99019 | | 19930729 | | |
| | WO 1994-US7989 | | 19940715 | | |
| | US 1994-313069 | | 19940926 | | |
| OS | MARPAT 128:114969 | | | | |
| GI | | | | | |



I



II

AB Title compds. [I, II; R1, R2 = H, halo, cyano, carboxamido, carboxy, carbamoyloxy, aminocarbonyl, formyloxy, formyl, azido, nitro, imidazolyl, ureido, thioureido, thiocyanato, OH, SH, sulfonamido, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, alkoxy, alkoxyalkyl, alkoxy carbonyl, aryloxy, acylamino, alkylsulfonylamino, alkylthiocarbonyl, alkylthio, etc.; Q = (substituted) amino, amidino, aminoalkyleneamino, iminoalkyleneimino, guanidino, heterocyclyl; L = C3-9 alkylene where any methylene group can be replaced by alkene, alkyne, aryl, heteroatom-contg. functional group; R18-R21 = H, alkyl, halo, alkyl, alkoxy, haloalkyl, cyano, carboxy, OH, alkoxy carbonyl, alkylsulfonylalkyl; R22 = OH, alkoxy, alkenyloxy, aryloxy, alkylaminoalkoxy, etc.; A1 = R1CN, NR25; A2 = CR2, N, SO2, SO, S, O, CO, COR26, CNR25; B1 = CR1, N, NR25, CO; B2 = CR2, NR25, SO2, SO, S, O, CO; B3 = CR1, CHR2, CO; R25 = H, OH, alkoxy, alkyl, cyano, haloalkyl, (CH2)mR1; m = 1-3; R26 = H, alkyl, aryl, aralkyl], were prepd. Thus, I [QL = p-[H2N(HN:)C]C6H4C.tplbond.C; R1, R2, R18-R21 = H; R22 = OH; A2A1 = MeC:CH] (prepn. given) inhibited platelet aggregation with IC50 = 0.093 .mu.M.

IT 167853-81-8P 167853-82-9P 167854-25-3P
 167854-27-5P 167854-29-7P 167854-65-1P
 167854-72-0P 167854-80-0P 167854-88-8P
 167855-32-5P 167855-44-9P 167855-45-0P
 201552-27-4P 201552-28-5P 201552-29-6P
 201552-47-8P 201552-49-0P 201552-51-4P
 201552-53-6P 201552-55-8P 201552-56-9P
 201552-57-0P 201552-58-1P 201552-59-2P
 201552-60-5P 201552-61-6P 201552-62-7P
 201552-64-9P 201552-65-0P 201552-66-1P
 201552-67-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of tricyclic benzodiazepines as inhibitors of the GPIIBIIIA receptor)

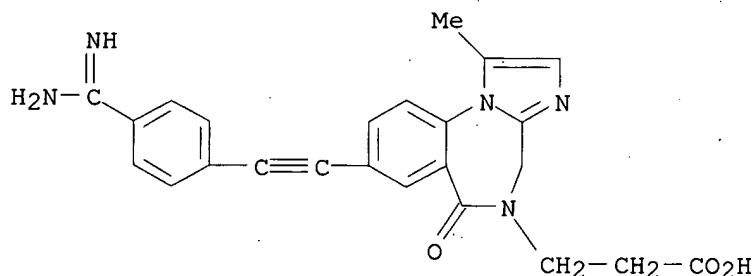
RN 167853-81-8 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, monoacetate (9CI)
 (CA INDEX NAME)

CM 1

CRN 167853-80-7

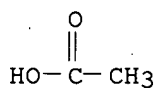
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CM 2

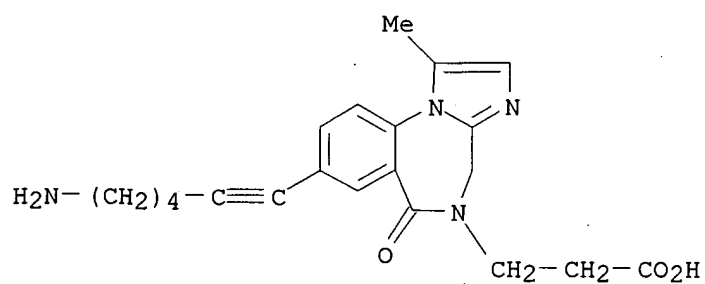
CRN 64-19-7

CMF C2 H4 O2



RN 167853-82-9 CAPLUS

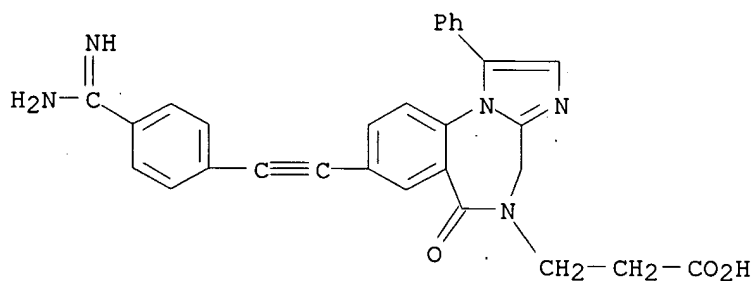
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-(6-amino-1-hexynyl)-1-methyl-6-oxo- (9CI) (CA INDEX NAME)



RN 167854-25-3 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)phenyl]ethynyl]-6-oxo-1-phenyl-, monoacetate (9CI)
 (CA INDEX NAME)

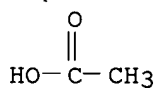
CM 1

CRN 167854-24-2
 CMF C29 H23 N5 O3



CM 2

CRN 64-19-7
 CMF C2 H4 O2

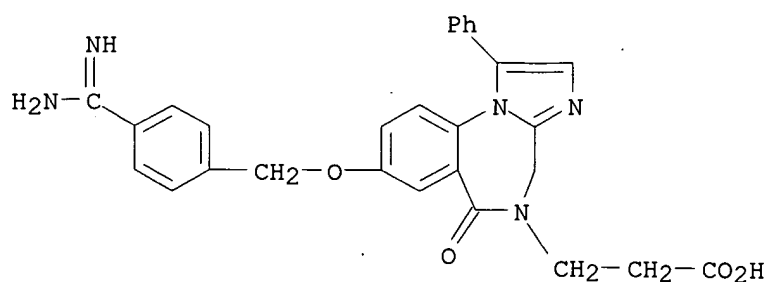


RN 167854-27-5 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)phenyl]methoxy]-6-oxo-1-phenyl-, monoacetate (9CI)
 (CA INDEX NAME)

CM 1

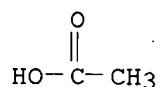
CRN 167854-26-4
 CMF C28 H25 N5 O4

09/868,356



CM 2

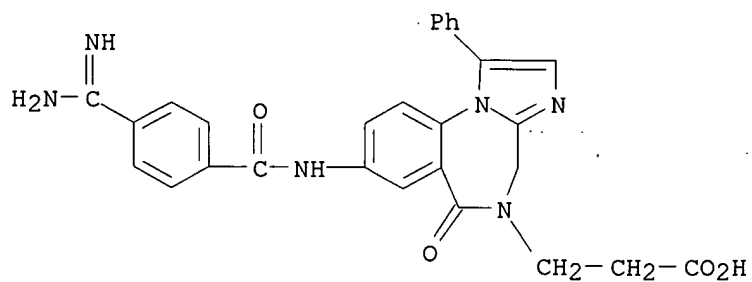
CRN 64-19-7
CMF C2 H4 O2



RN 167854-29-7 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-6-oxo-1-phenyl-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

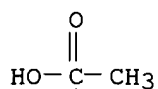
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CMF C28 H24 N6 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

09/868,356

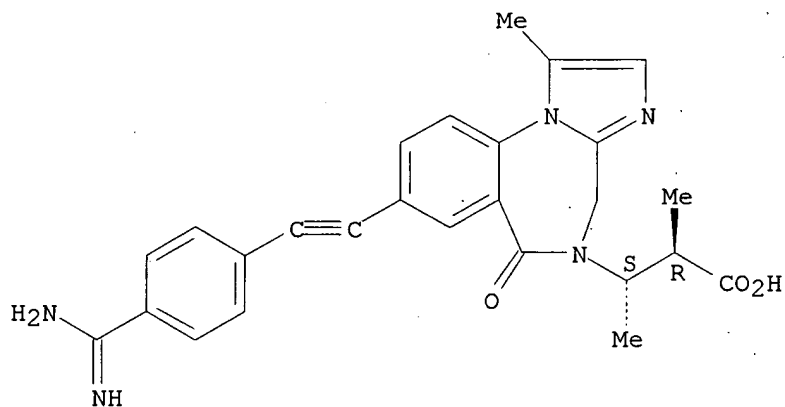


RN 167854-65-1 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-oxo-,
[S-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

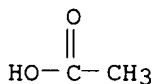
CRN 167854-64-0
CMF C26 H25 N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



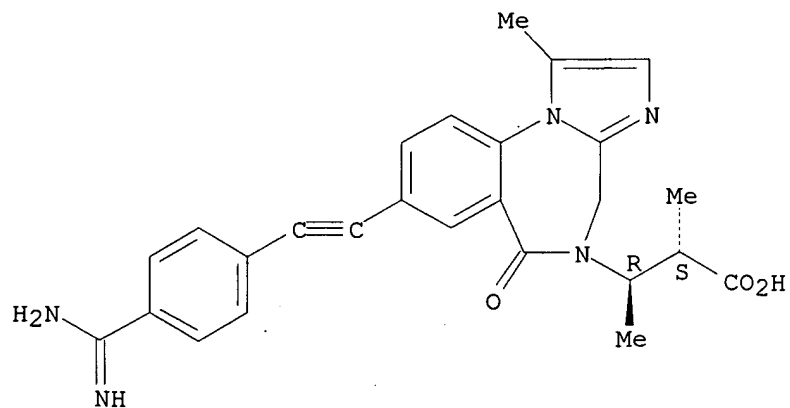
RN 167854-72-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-oxo-,
[R-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-71-9
CMF C26 H25 N5 O3

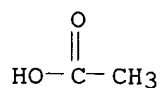
Absolute stereochemistry.

09/868,356



CM 2

CRN 64-19-7
CMF C2 H4 O2

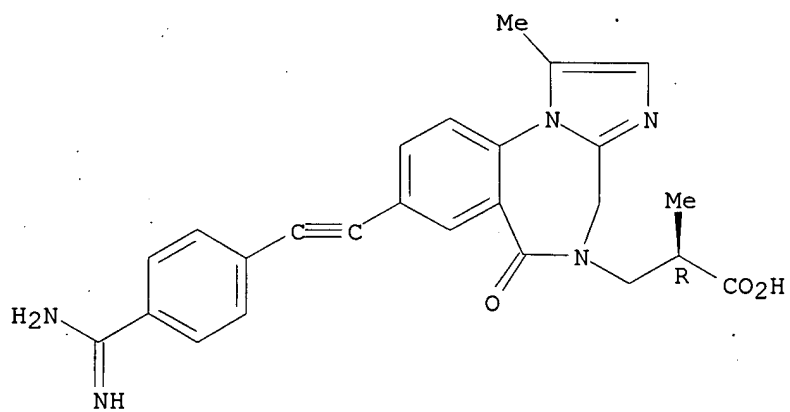


RN 167854-80-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-, (R)-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-79-7
CMF C25 H23 N5 O3

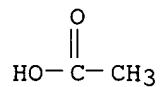
Absolute stereochemistry.



CM 2

09/868,356

CRN 64-19-7
CMF C2 H4 O2

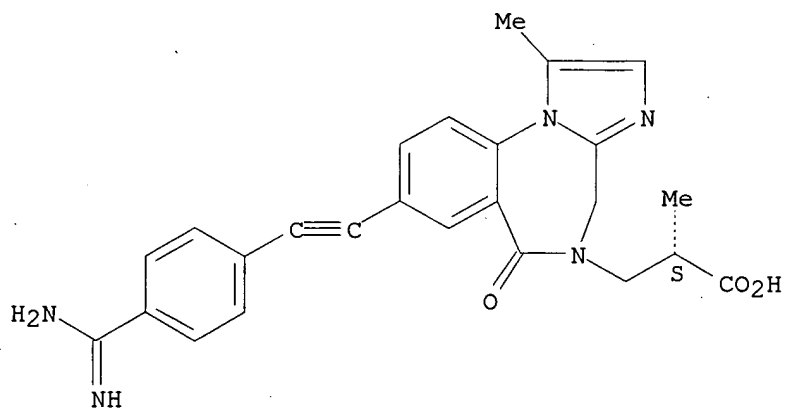


RN 167854-88-8 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-, (S)-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

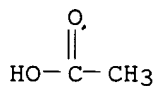
CRN 167854-87-7
CMF C25 H23 N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



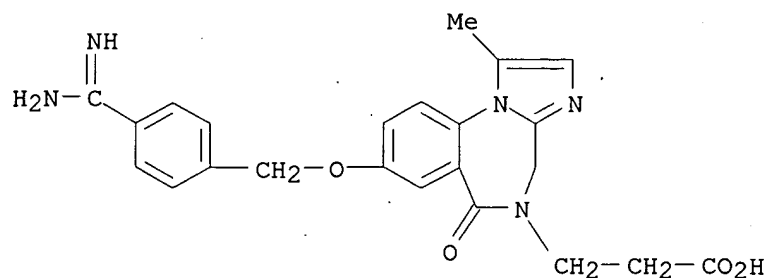
RN 167855-32-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]methoxy]-1-methyl-6-oxo-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

CRN 167855-31-4

09/868,356

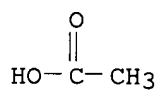
CMF C23 H23 N5 O4



CM 2

CRN 64-19-7

CMF C2 H4 O2



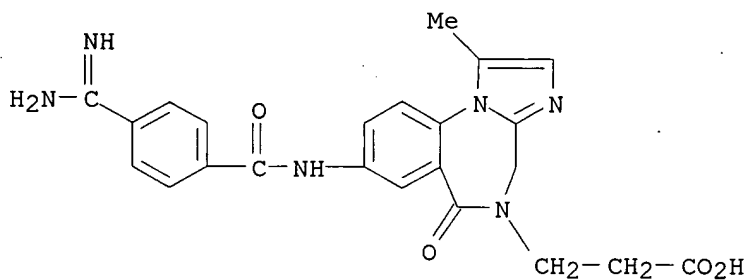
RN 167855-44-9 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167855-43-8

CMF C23 H22 N6 O4

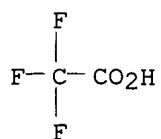


CM 2

CRN 76-05-1

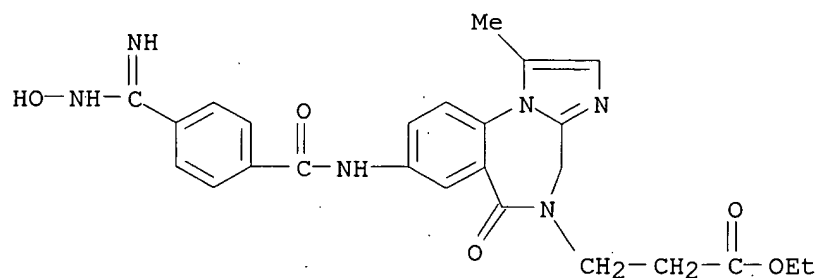
CMF C2 H F3 O2

09/868,356



RN 167855-45-0 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-[(hydroxyamino)iminomethyl]benzoyl]amino]-1-methyl-6-oxo-, ethyl
ester (9CI) (CA INDEX NAME)



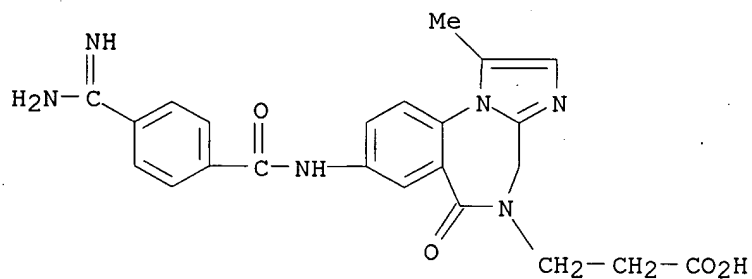
RN 201552-27-4 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

CRN 167855-43-8

CMF C23 H22 N6 O4

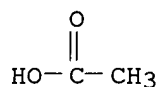


CM 2

CRN 64-19-7

CMF C2 H4 O2

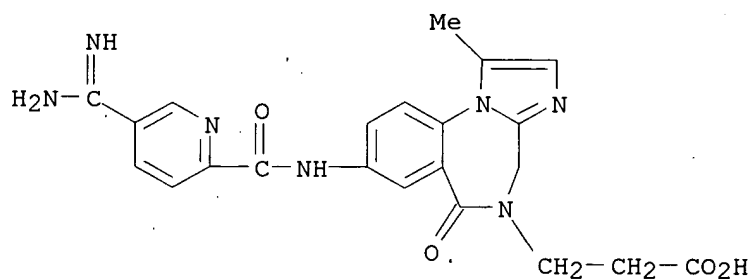
09/868,356



RN 201552-28-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[[5-(aminoiminomethyl)-2-pyridinyl]carbonyl]amino]-1-methyl-6-oxo-,
monoacetate (9CI) (CA INDEX NAME)

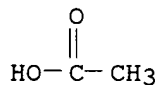
CM 1

CRN 167854-22-0
CMF C22 H21 N7 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

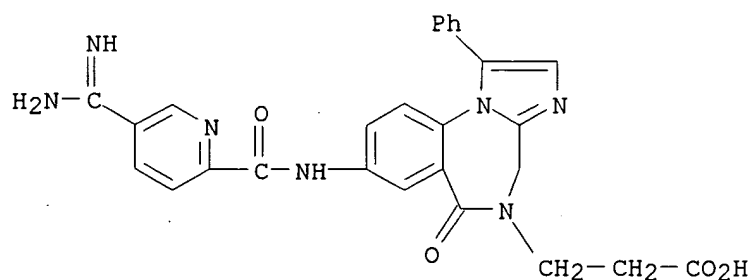


RN 201552-29-6 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[[5-(aminoiminomethyl)-2-pyridinyl]carbonyl]amino]-6-oxo-1-phenyl-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

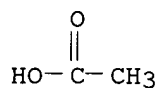
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09/868,356



CM 2

CRN 64-19-7
CMF C2 H4 O2

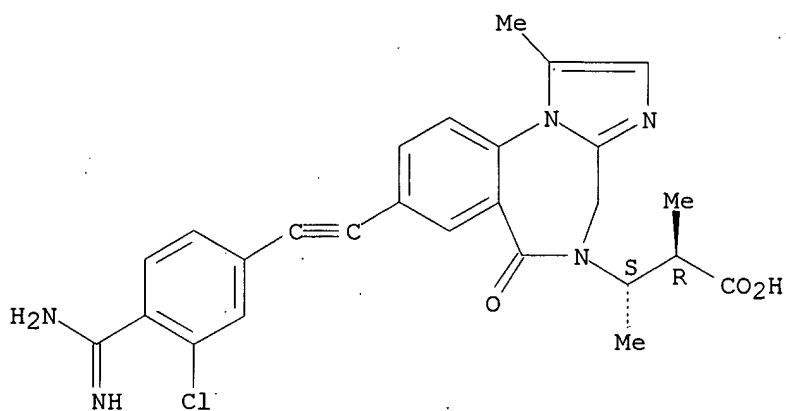


RN 201552-47-8 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,.beta.,1-
trimethyl-6-oxo-, [S-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 201552-46-7
CMF C26 H24 Cl N5 O3

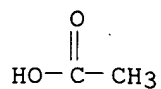
Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

09/868,356

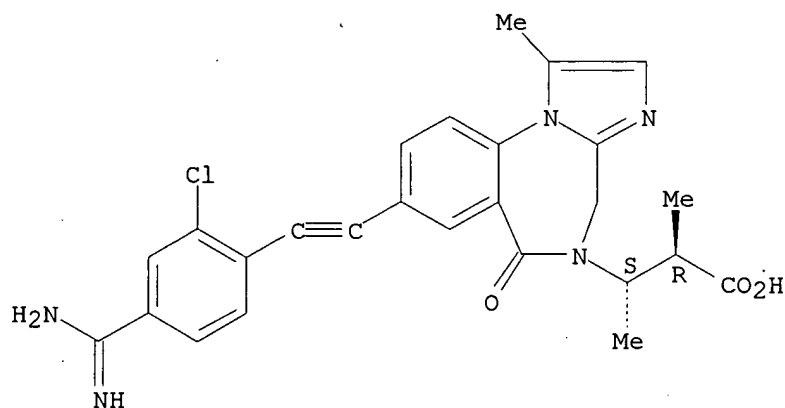


RN 201552-49-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,.beta.,1-
trimethyl-6-oxo-, [S-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

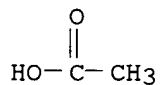
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CMF C26 H24 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

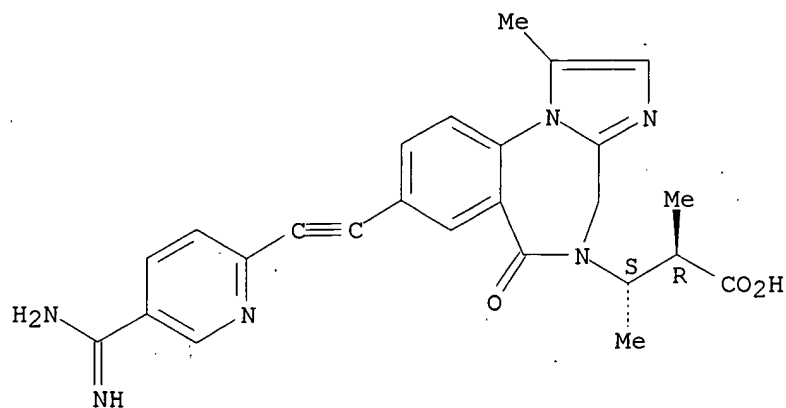


RN 201552-51-4 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-
oxo-, [S-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 201552-50-3
CMF C25 H24 N6 O3

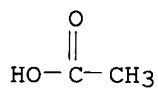
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 201552-53-6 CAPLUS

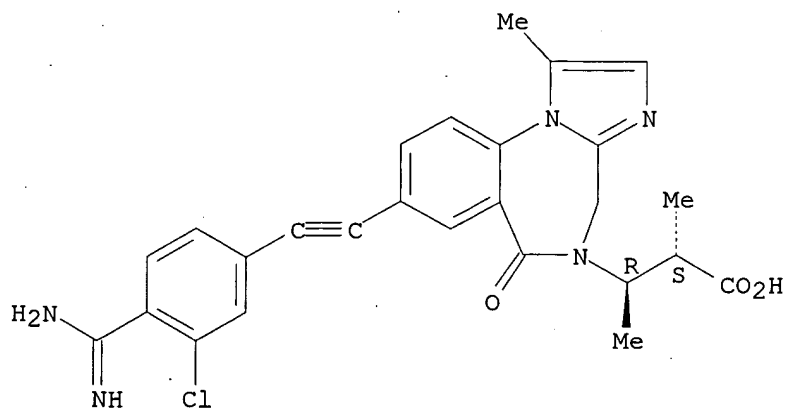
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,.beta.,1-
trimethyl-6-oxo-, [R-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 201552-52-5

CMF C26 H24 Cl N5 O3

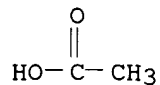
Absolute stereochemistry.



09/868,356

CM 2

CRN 64-19-7
CMF C2 H4 O2

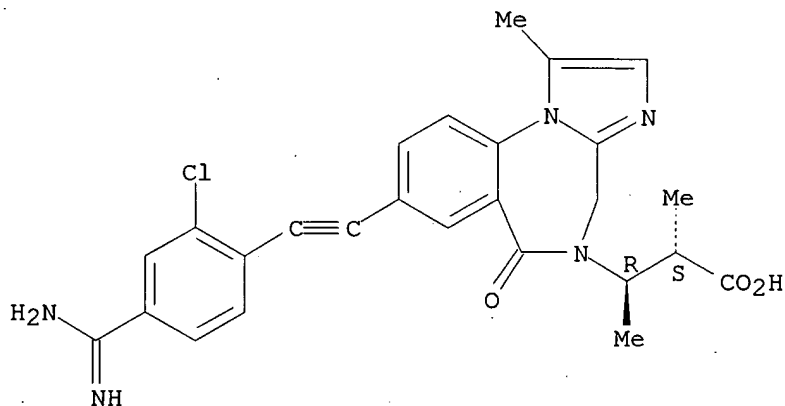


RN 201552-55-8 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,.beta.,1-
trimethyl-6-oxo-, [R-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

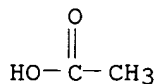
CRN 201552-54-7
CMF C26 H24 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



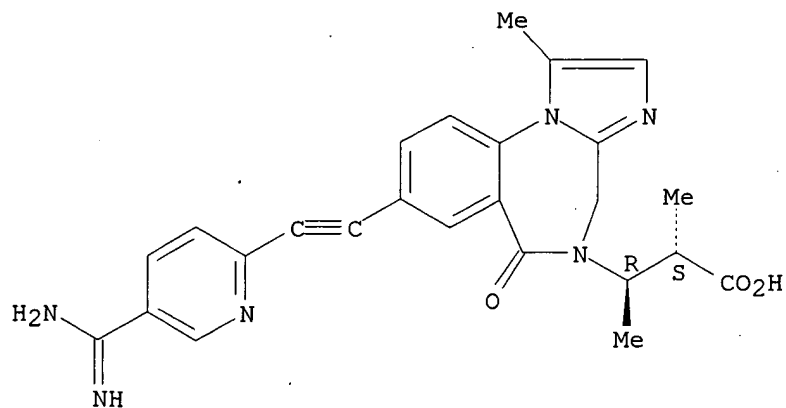
RN 201552-56-9 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-
oxo-, [R-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

09/868,356

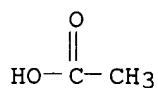
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CMF C25 H24 N6 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

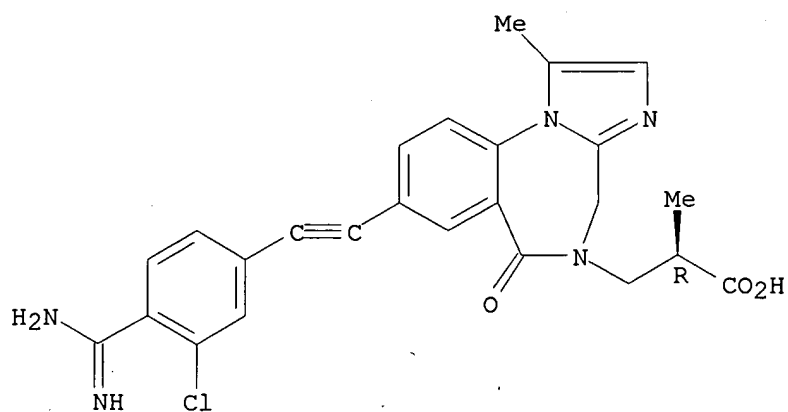


RN 201552-57-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-
, (R)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-81-1
CMF C25 H22 Cl N5 O3

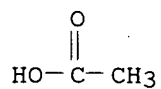
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 201552-58-1 CAPLUS

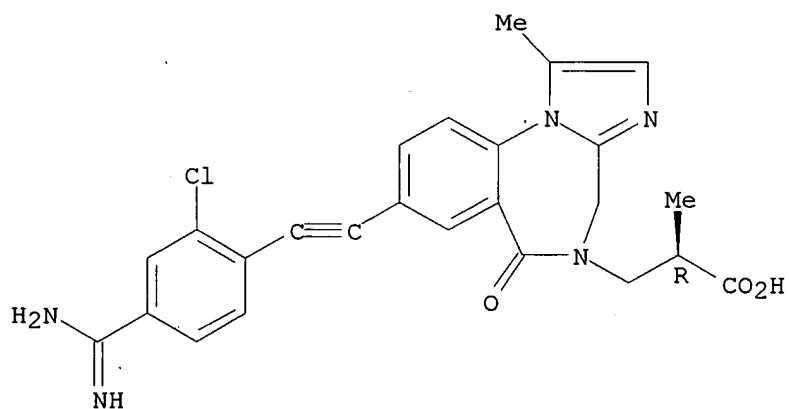
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-
, (R)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-83-3

CMF C25 H22 Cl N5 O3

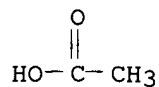
Absolute stereochemistry.



09/868,356

CM 2

CRN 64-19-7
CMF C2 H4 O2

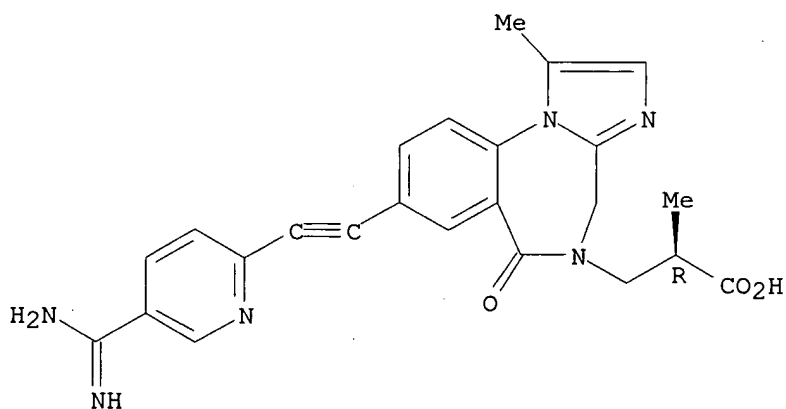


RN 201552-59-2 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-,
(R)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

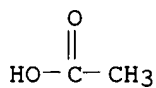
CRN 167854-85-5
CMF C24 H22 N6 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



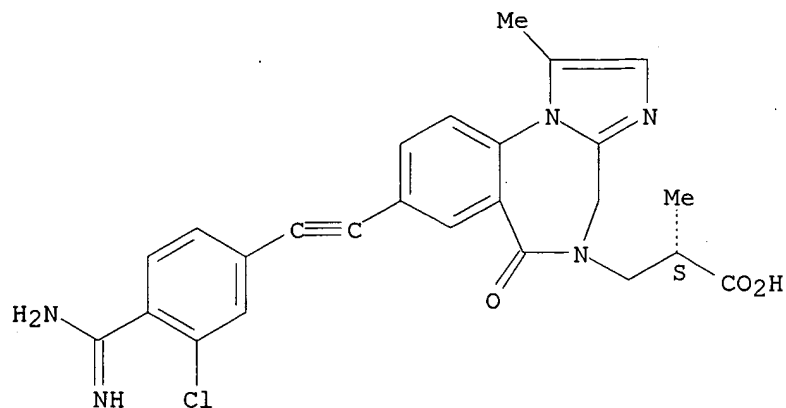
RN 201552-60-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-,
(S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

09/868,356

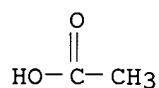
CRN 167854-89-9
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

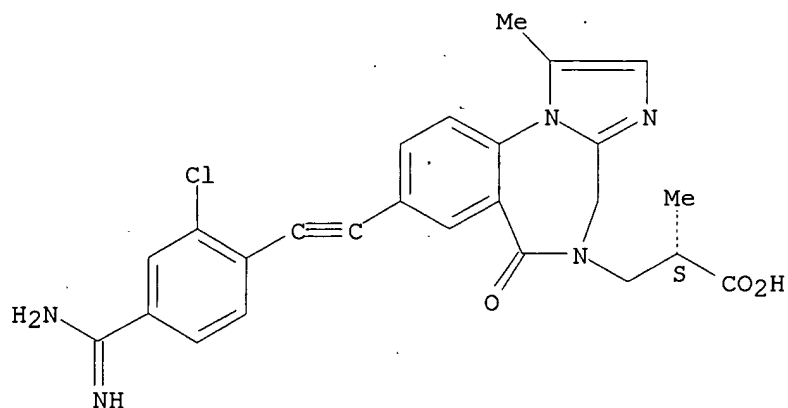


RN 201552-61-6 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-
, (S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-91-3
CMF C25 H22 Cl N5 O3

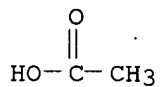
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 201552-62-7 CAPLUS

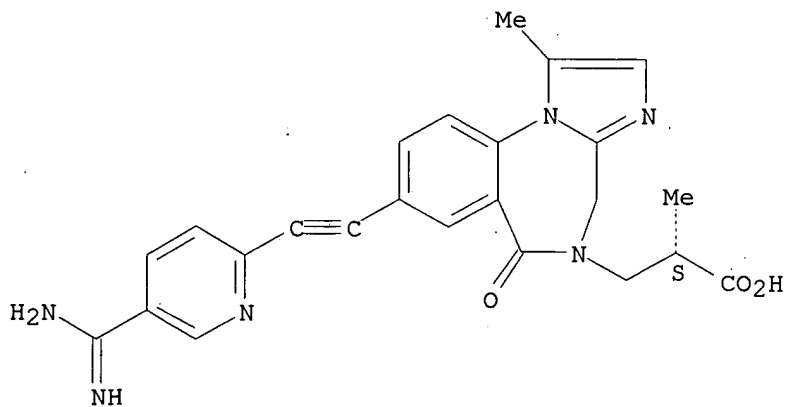
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-,
(S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-93-5

CMF C24 H22 N6 O3

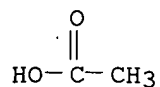
Absolute stereochemistry.



09/868,356

CM 2

CRN 64-19-7
CMF C2 H4 O2

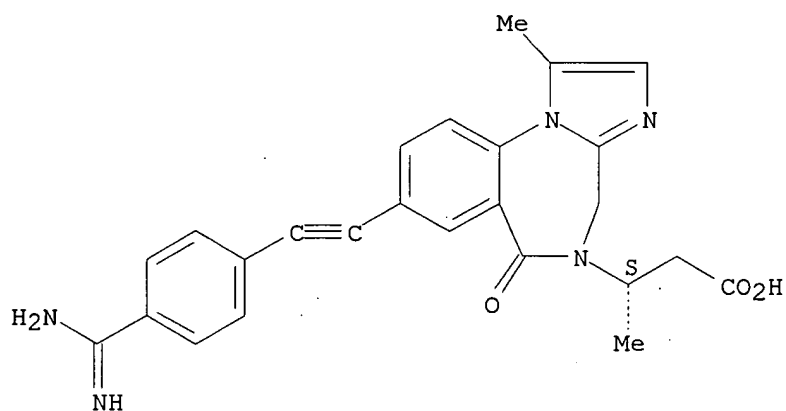


RN 201552-64-9 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.beta.,1-dimethyl-6-oxo-, (S)-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

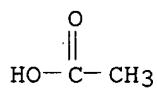
CRN 201552-63-8
CMF C25 H23 N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



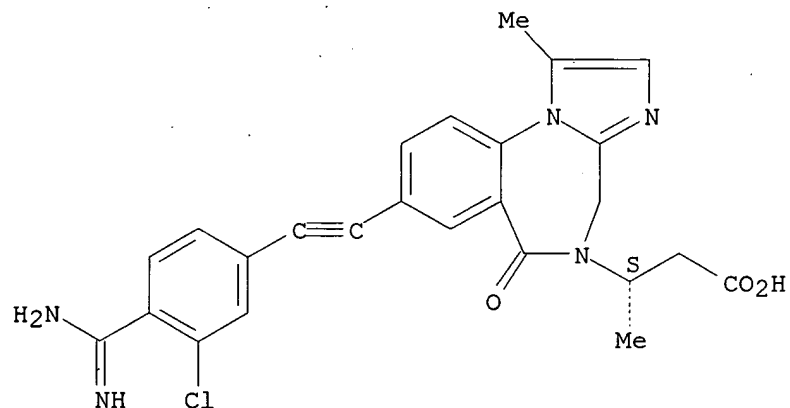
RN 201552-65-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

09/868,356

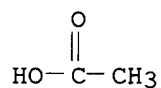
CRN 167854-95-7
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



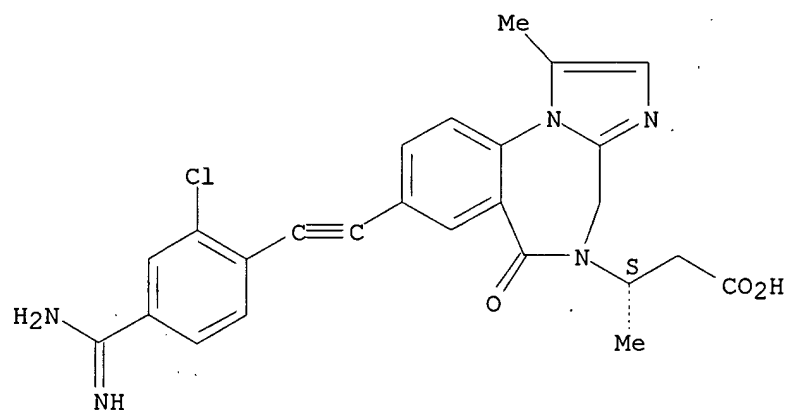
RN 201552-66-1 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-97-9
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.

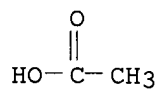
09/868,356



CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 201552-67-2 CAPLUS

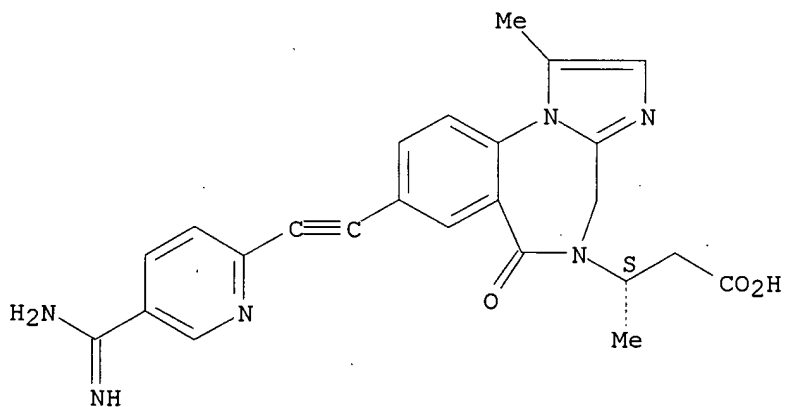
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-99-1

CMF C24 H22 N6 O3

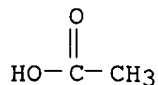
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2



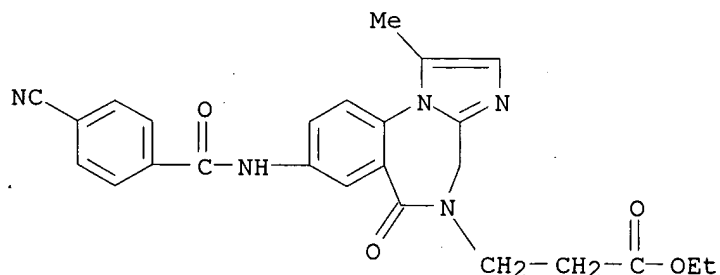
IT 167853-92-1P 167853-94-3P 167853-96-5P
 167853-97-6P 167854-00-4P 167854-14-0P
 167854-16-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of tricyclic benzodiazepines as inhibitors of the GPIIBIIIA
 receptor)

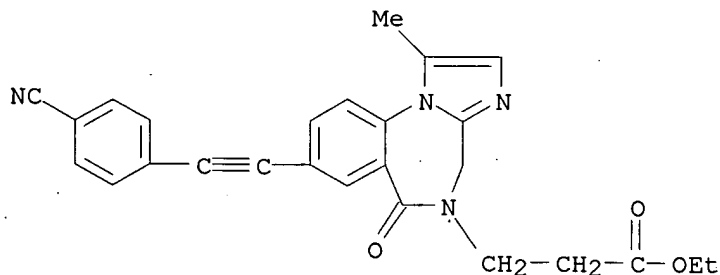
RN 167853-92-1 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[(4-cyanobenzoyl)amino]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
 NAME)



RN 167853-94-3 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[(4-cyanophenyl)ethynyl]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
 NAME)



RN 167853-96-5 CAPLUS

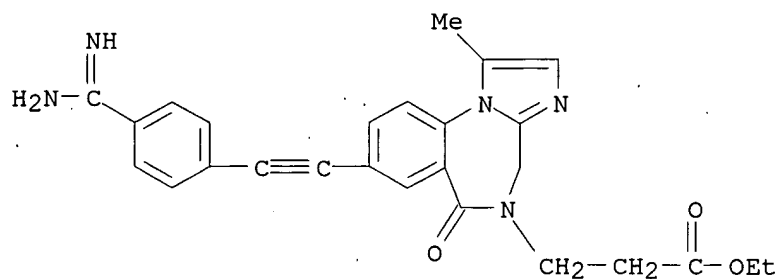
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, ethyl ester,
 monoacetate (9CI) (CA INDEX NAME)

09/868,356

CM 1

CRN 167853-95-4

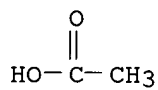
CMF C26 H25 N5 O3



CM 2

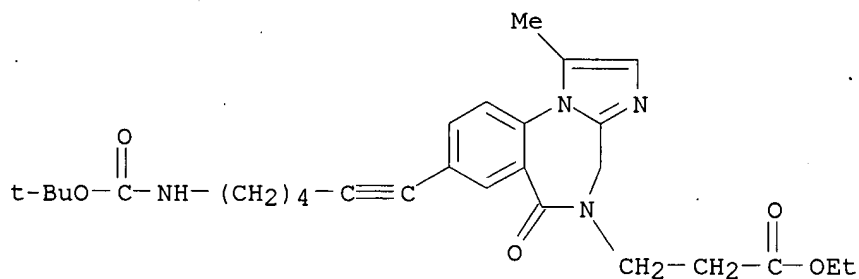
CRN 64-19-7

CMF C2 H4 O2



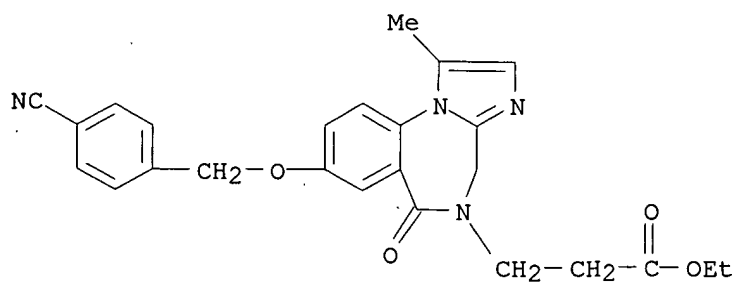
RN 167853-97-6 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[6-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-hexynyl]-1-methyl-6-oxo-,
ethyl ester (9CI) (CA INDEX NAME)

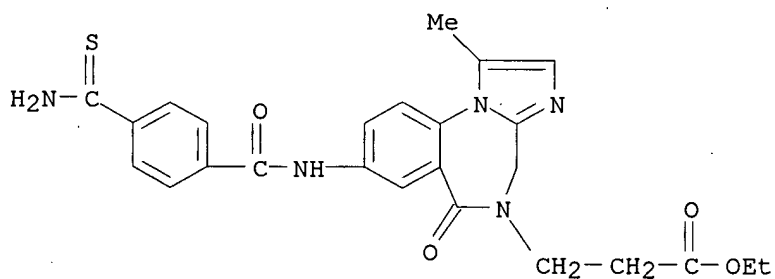


RN 167854-00-4 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[(4-cyanophenyl)methoxy]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
NAME)



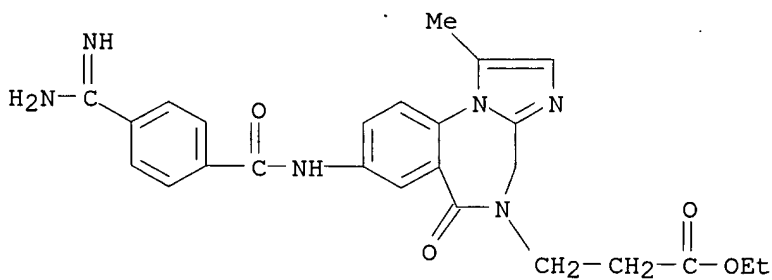
RN 167854-14-0 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminothioxomethyl)benzoyl]amino]-1-methyl-6-oxo-, ethyl ester (9CI)
 (CA INDEX NAME)



RN 167854-16-2 CAPLUS
 CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
 8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-, ethyl ester,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-15-1
 CMF C25 H26 N6 O4

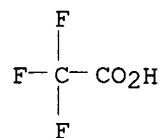


CM 2

CRN 76-05-1

09/868,356

CMF C2 H F3 O2

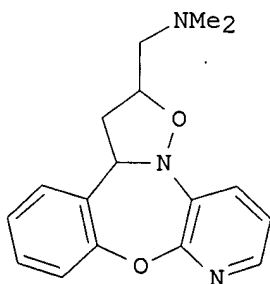
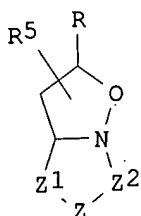


RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/868,356

127 ANSWER 14 OF 46 CAPLUS COPYRIGHT 2003 ACS
AN 1997:732208 CAPLUS
DN 127:346383
TI Preparation of anellated isoxazolidinemethanamines and analogs as 5-HT antagonists
IN Andres Gil, Jose Ignacio; Martinez, Pedro; Fernandez Gadea, Francisco Javier; Sipido, Victor Karel
PA Janssen Pharmaceutica N.V., Belg.
SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|--|----------|-----------------|----------|
| PI | WO 9739001 | A1 | 19971023 | WO 1997-EP1830 | 19970409 |
| | W: | AL, AM, AU, BB, BG, BR, CA, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, LC, LK, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, TJ, TM | | | |
| | RW: | GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | |
| | CA 2232195 | AA | 19971023 | CA 1997-2232195 | 19970409 |
| | AU 9723852 | A1 | 19971107 | AU 1997-23852 | 19970409 |
| | AU 716470 | B2 | 20000224 | | |
| | CN 1205010 | A | 19990113 | CN 1997-191421 | 19970409 |
| | CN 1082963 | B | 20020417 | | |
| | EP 892804 | A1 | 19990127 | EP 1997-919344 | 19970409 |
| | EP 892804 | B1 | 20020828 | | |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | |
| | JP 2000508328 | T2 | 20000704 | JP 1997-536734 | 19970409 |
| | IL 123656 | A1 | 20010913 | IL 1997-123656 | 19970409 |
| | AT 222911 | E | 20020915 | AT 1997-919344 | 19970409 |
| | HU 221608 | B | 20021128 | HU 1999-1875 | 19970409 |
| | ES 2182064 | T3 | 20030301 | ES 1997-919344 | 19970409 |
| | ZA 9703122 | A | 19981012 | ZA 1997-3122 | 19970411 |
| | NO 9801077 | A | 19981012 | NO 1998-1077 | 19980311 |
| | US 6156747 | A | 20001205 | US 1998-155839 | 19981006 |
| PRAI | EP 1996-200991 | A | 19960412 | | |
| | WO 1997-EP1830 | W | 19970409 | | |
| OS | MARPAT 127:346383 | | | | |
| GI | | | | | |



AB Title compds. [I; R = (CH₂)_nNR₁R₂; R₁,R₂ = H, alkyl, alkanoyl, etc.; NR₁R₂ = heterocyclcyl; R₅ = H or 1-3 of alkyl, cyano, trihalomethyl; Z = (un)substituted CH₂, (alkyl)imino, O, SOO-2; Z₁,Z₂ = (un)substituted heteroarylene, 1,2-phenylene, etc.; n = 0-6] were prepd. Thus, 2-(HO)C₆H₄CHO was etherified by 2-chloro-3-nitropyridine and the product cyclized to give pyrido[2,3-b][1,4]benzoxazepine 5-oxide which was cyclocondensed with 3-amino-1-propene (sic) to give title compd. cis-II. Data for biol. activity of I were given.

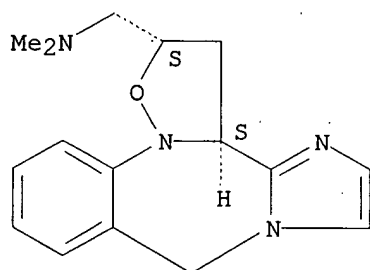
IT **198343-97-4P 198344-12-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of anellated isoxazolidinemethanamines and analogs as 5-HT antagonists)

RN 198343-97-4 CAPLUS

CN 2H,8H-Imidazo[2,1-c]isoxazolo[2,3-a][1,4]benzodiazepine-2-methanamine, 3,3a-dihydro-N,N-dimethyl-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

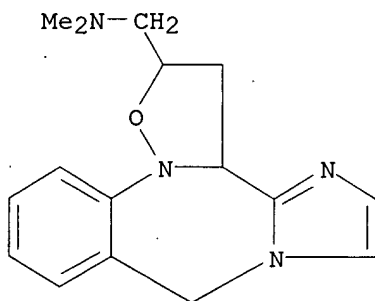
Relative stereochemistry.



● 2 HCl

RN 198344-12-6 CAPLUS

CN 2H,8H-Imidazo[2,1-c]isoxazolo[2,3-a][1,4]benzodiazepine-2-methanamine, 3,3a-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



~~L2~~ ANSWER 15 OF 46 CAPLUS COPYRIGHT 2003 ACS

~~AN~~ 1997:547298 CAPLUS

DN 127:149074

TI Pyridine derivatives and analogs useful as vitronectin receptor antagonists

IN Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James

PA Smithkline Beecham Corporation, USA; Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James

SO PCT Int. Appl., 123 pp.

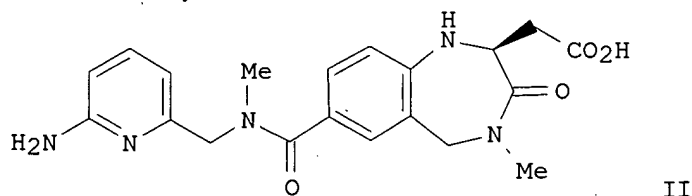
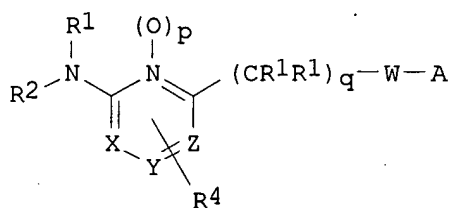
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9724122 | A1 | 19970710 | WO 1996-US20744 | 19961220 |
| | W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2241724 | AA | 19970710 | CA 1996-2241724 | 19961220 |
| | AU 9713538 | A1 | 19970728 | AU 1997-13538 | 19961220 |
| | EP 895475 | A1 | 19990210 | EP 1996-945085 | 19961220 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI | | | | |
| | CN 1209060 | A | 19990224 | CN 1996-180099 | 19961220 |
| | BR 9612378 | A | 19990713 | BR 1996-12378 | 19961220 |
| | JP 2000502708 | T2 | 20000307 | JP 1997-524556 | 19961220 |
| | ZA 9610855 | A | 19971124 | ZA 1996-10855 | 19961223 |
| | NO 9803002 | A | 19980826 | NO 1998-3002 | 19980626 |
| | US 2001034445 | A1 | 20011025 | US 2001-769125 | 20010124 |
| PRAI | US 1995-9532P | P | 19951229 | | |
| | WO 1996-US20744 | W | 19961220 | | |
| | US 1998-91936 | B1 | 19981203 | | |
| OS | MARPAT 127:149074 | | | | |
| GI | | | | | |



AB Title compds. I [A = fibrinogen antagonist template; W = (CHR3)nU(CHR3)mV; X, Y, Z = N or CR4, provided that at most one is N; R1 = H, alkyl, cycloalkyl(alkyl), aryl(alkyl); R2 = R1, COR1, CO2R1; R3 = H, alkyl, heterocycl(alkyl), cycloalkyl(alkyl), aryl(alkyl); R4 = H, halo, OR3, SR3, cyano, (un)substituted NH2, etc.; U, V = bond, CO, CR3R3, S, SO, SO2, O, NR3, etc.; n, m = 0, 1, 2; p, q = 0, 1; with addnl. provisos] are disclosed. The compds. are vitronectin receptor antagonists, useful in the treatment of osteoporosis and other conditions. I are said to inhibit binding of SKF 107260 to vitronectin receptor in vitro at 0.01 to 25 .mu.M, with some compds. showing at least a 4-fold (and in some cases 10-fold) greater affinity for vitronectin receptor over fibrinogen receptor. Examples include prepn. of 35 title compds., with characterizing data for 4 of them. For instance, amidation of 6-[(methylamino)methyl]-2-pyridinamine with the corresponding carboxybenzodiazepineacetate deriv., and sapon. of the product with LiOH in aq. THF, gave title compd. II.

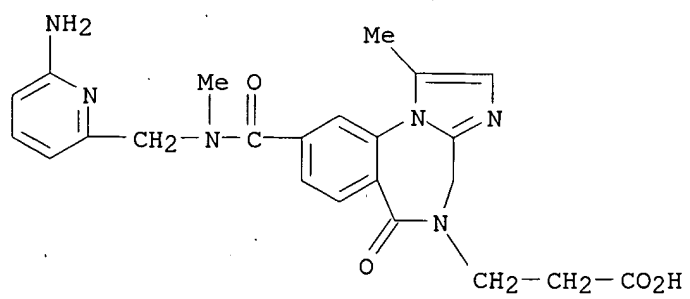
IT **193469-89-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyridine derivs. and analogs as vitronectin receptor antagonists)

RN 193469-89-5 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
9-[[[(6-amino-2-pyridinyl)methyl]methylamino]carbonyl]-1-methyl-6-oxo-
(9CI) (CA INDEX NAME)



~~127~~ ANSWER 16 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1997:547296 CAPLUS

DN 127:161822

TI Benzimidazole derivatives and analogs as vitronectin receptor antagonists.

IN Miller, William Henry; Bondinell, William Edward; Ku, Thomas Wen-fu; Keenan, Richard Mcculloch; Samanen, James Martin; Kwon, Chet; Ali, Fadia El-fehail; Lago, Maria A.

PA Smithkline Beecham Corporation, USA; Miller, William Henry; Bondinell, William Edward; Ku, Thomas Wen-Fu; Keenan, Richard Mcculloch; Samanen, James Martin; Kwon, Chet; Ali, Fadia El-Fehail; Lago, Maria A.

SO PCT Int. Appl., 238 pp.

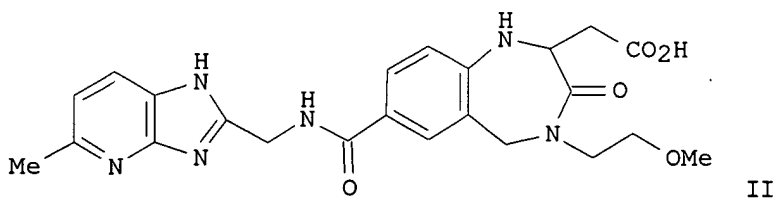
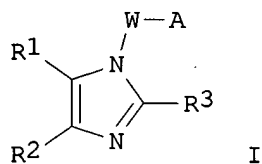
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|--|----------|-----------------|----------|
| PI | WO 9724119 | A1 | 19970710 | WO 1996-US20748 | 19961220 |
| | W: | AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | |
| | CA 2241633 | AA | 19970710 | CA 1996-2241633 | 19961220 |
| | AU 9713540 | A1 | 19970728 | AU 1997-13540 | 19961220 |
| | EP 869787 | A1 | 19981014 | EP 1996-945087 | 19961220 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | |
| | CN 1209744 | A | 19990303 | CN 1996-180113 | 19961220 |
| | BR 9612327 | A | 19990713 | BR 1996-12327 | 19961220 |
| | JP 2000502354 | T2 | 20000229 | JP 1997-524557 | 19961220 |
| | ZA 9610859 | A | 19971024 | ZA 1996-10859 | 19961223 |
| | NO 9803003 | A | 19980826 | NO 1998-3003 | 19980626 |
| PRAI | US 1995-9366P | P | 19951229 | | |
| | WO 1996-US20748 | W | 19961220 | | |
| OS | MARPAT 127:161822 | | | | |
| GI | | | | | |



AB A variety of imidazoles, benzimidazoles, and analogs are disclosed, e.g., I [W = XV or C₆H₄; X = bond, (un)substituted CH₂ or CH₂CH₂; V = certain substituted CONH or NHCO linkages; R₁, R₂ = H, alkyl, aralkyl, heteroaralkyl, halo, CF₃, etc.; or R₁R₂ forms (un)substituted 5- or 6-membered carbo- or heterocyclic ring; R₃ = H, alkyl, aralkyl; A = fibrinogen receptor antagonist template]. The compds. are vitronectin receptor antagonists, useful in the treatment of osteoporosis. Invention compds. are said to inhibit binding of SKF 107260 to vitronectin receptor at 0.001 to 50 μ M, and to have a vitronectin receptor K_i approx. 10- to 100-fold greater than that at the fibrinogen receptor. Over 80 example compds. are given, with characterization of 59 compds. For instance, title compd. II was prepd. by amidation of 2-(aminomethyl)-4-aza-5-methylbenzimidazole di-HCl with the corresponding carboxybenzodiazepineacetate deriv., using EDC and HOBt, followed by sapon. with LiOH in aq. THF.

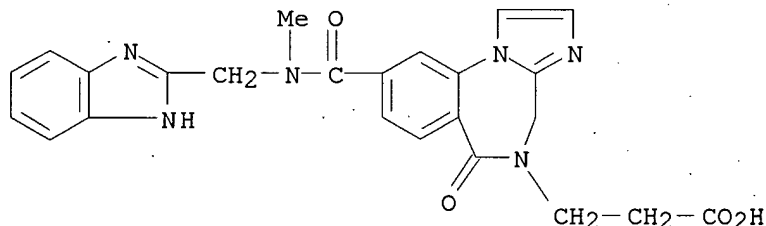
IT **193532-92-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazole derivs. and analogs as vitronectin receptor antagonists)

RN 193532-92-2 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 9-[[[(1H-benzimidazol-2-ylmethyl)methylamino]carbonyl]-6-oxo- (9CI) (CA INDEX NAME)



~~127~~ ANSWER 17 OF 46 CAPLUS COPYRIGHT 2003 ACS

~~AN~~ 1997:547292 CAPLUS

DN 127:149073

TI Pyridine derivatives and analogs useful as vitronectin receptor antagonists

IN Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James

PA Smithkline Beecham Corporation, USA; Ali, Fadia E.; Bondinell, William E.; Keenan, Richard M.; Ku, Thomas Wen Fu; Miller, William H.; Samanen, James

SO PCT Int. Appl., 133 pp.

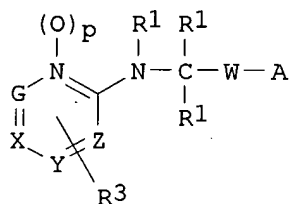
CODEN: PIXXD2

DT Patent

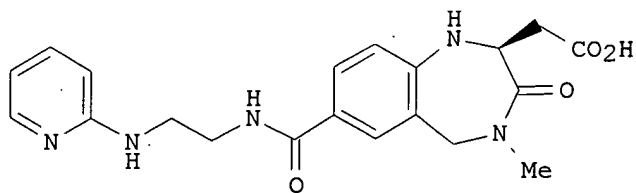
LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9724124 | A1 | 19970710 | WO 1996-US20327 | 19961220 |
| | W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| | AU 9712955 | A1 | 19970728 | AU 1997-12955 | 19961220 |
| | CN 1209063 | A | 19990224 | CN 1996-180114 | 19961220 |
| | EP 906103 | A1 | 19990407 | EP 1996-943818 | 19961220 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI | | | | |
| | BR 9612381 | A | 19990713 | BR 1996-12381 | 19961220 |
| | JP 2000502704 | T2 | 20000307 | JP 1997-524453 | 19961220 |
| | ZA 9610854 | A | 19980402 | ZA 1996-10854 | 19961223 |
| | NO 9803001 | A | 19980826 | NO 1998-3001 | 19980626 |
| | US 6159964 | A | 20001212 | US 1999-91937 | 19990727 |
| PRAI | US 1995-9367P | P | 19951229 | | |
| | WO 1996-US20327 | W | 19961220 | | |
| OS | MARPAT 127:149073 | | | | |
| GI | | | | | |



I



II

AB Title compds. I [A = fibrinogen antagonist template; W = (CHR₂)_nU(CHR₂)_mV; G, X, Y, Z = N or CR₃, provided that no more than one is N; R₁ = H, alkyl, cycloalkyl(alkyl), aryl(alkyl); R₂ = H, alkyl, heterocycl(alkyl), cycloalkyl(alkyl), aryl(alkyl); R₃ = H, halo, OR₂, SR₂, cyano, (un)substituted NH₂, etc.; U, V = bond, CO, CR₂R₂, S, SO, SO₂, O, NR₂, etc.; n = 0, 1, 2, 3; m = 0, 1, 2; p = 0, 1] are disclosed. The compds. are vitronectin receptor antagonists, useful in the treatment of osteoporosis and other conditions. I are said to inhibit binding of SKF 107260 to vitronectin receptor in vitro at 0.01 to 25 .mu.M, with some compds. showing at least a 4-fold (and in some cases 10-fold) greater affinity for vitronectin receptor over fibrinogen receptor. Examples include preps. of 41 title compds., with characterizing data for several of them. For instance, amidation of N-(2-pyridinyl)ethylenediamine with the corresponding carboxybenzodiazepineacetate deriv., and sapon. of the product with LiOH in aq. THF, gave title compd. II.

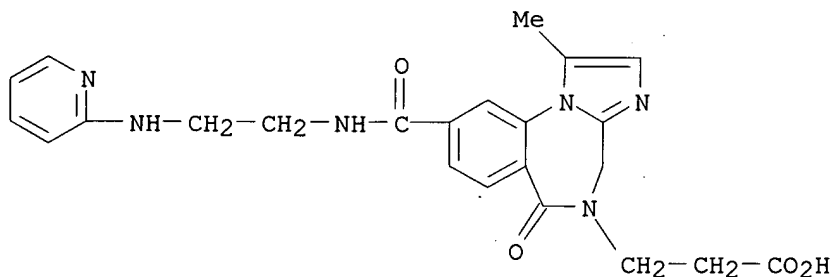
IT 193473-21-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

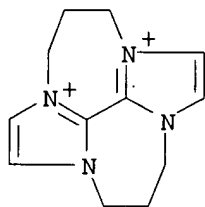
(prepn. of pyridine derivs. and analogs as vitronectin receptor antagonists)

RN 193473-21-1 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 1-methyl-6-oxo-9-[[[2-(2-pyridinylamino)ethyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



~~LE~~7 ANSWER 18 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1997:540524 CAPLUS
 DN 127:212412
 TI Optical and Thermal Electron Transfer Activation of Dioxygen by Viologen Dithiolene Metalates
 AU Ammon, U.; Chiorboli, C.; Duemler, W.; Grampp, G.; Scandola, F.; Kisch, H.
 CS Institut fuer Anorganische Chemie, Universitaet Erlangen-Nuernberg, Erlangen, D-91058, Germany
 SO Journal of Physical Chemistry A (1997), 101(37), 6876-6882
 CODEN: JPCAFH; ISSN: 1089-5639
 PB American Chemical Society
 DT Journal
 LA English
 AB Photoinduced electron transfer activation of dioxygen by redoxactive charge-transfer ion pairs of the type $\{A_2^+[Pt(mnt)_2]^{2-}\}$ ($A_2^+ = 2,2'$ -, $4,4'$ -bipyridinium or cycloalkylated biimidazolium dication; $mnt =$ maleonitriledithiolate) occurs through an optical electron transfer within an ion pair. This affords the primary redox products A_{bul}^+ and $[Pt(mnt)_2]^-$ as indicated by laser flash photolysis. Under argon the transients recombine by fast second-order kinetics. Under dioxygen a different behavior is obsd. In the case of acceptors with a first redn. potential more pos. than -0.6 V back electron transfer prevails. When the potential is more neg. however, A_{bul}^+ reduces O_2 by pseudo-first-order kinetics to generate $O_{2\text{bul}}^-$, while $[Pt(mnt)_2]^-$ accumulates in the soln. Quantum yields increase with decreasing excitation wavelength. This suggests that internal conversion of the initially populated excited state to the photoreactive ion pair charge-transfer state is more efficient upon excitation to the interligand (π ., π *) state (334 nm) than to the metal-to-ligand charge-transfer state (437 or 580 nm). In the latter cases competitive radiationless deactivation via metal-centered states occurs. The corresponding Ni and Pd complexes do not exhibit any reactivity due to their very short excited state lifetimes. Formation of $O_{2\text{bul}}^-$ was proved by ESR spin-trapping techniques. Accumulation of $[Pt(mnt)_2]^-$ occurs also when instead of irradiating, the reaction is performed in the dark at about 160°C . The activation energy of 108 ± 10 kJ/mol as obtained for the thermal electron transfer from $[Pt(mnt)_2]^{2-}$ to A_2^+ corresponds well to the value calcd. from the Hush-Marcus model.
 IT **162477-59-0**
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (photochem. and thermal electron transfer reaction of mol. oxygen by viologen dithiolene metalate ion pairs contg.)
 RN 162477-59-0 CAPLUS
 CN 3H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene, 4,5,9,10-tetrahydro- (9CI) (CA INDEX NAME)



~~L27~~ ANSWER 19 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1997:156150 CAPLUS

DN 126:264038

TI Annulated derivatives of 2,2'-biimidazole, 2-(2'-imidazolyl)benzimidazole, and 2,2'-bibenzimidazole

AU Ames, James R.; Houghtaling, Melissa A.; Terrian, Deborah L.; Mitchell, Timothy P.

CS Department Chemistry, University Michigan-Flint, Flint, MI, 48502-2186, USA

SO Canadian Journal of Chemistry (1997), 75(1), 28-36

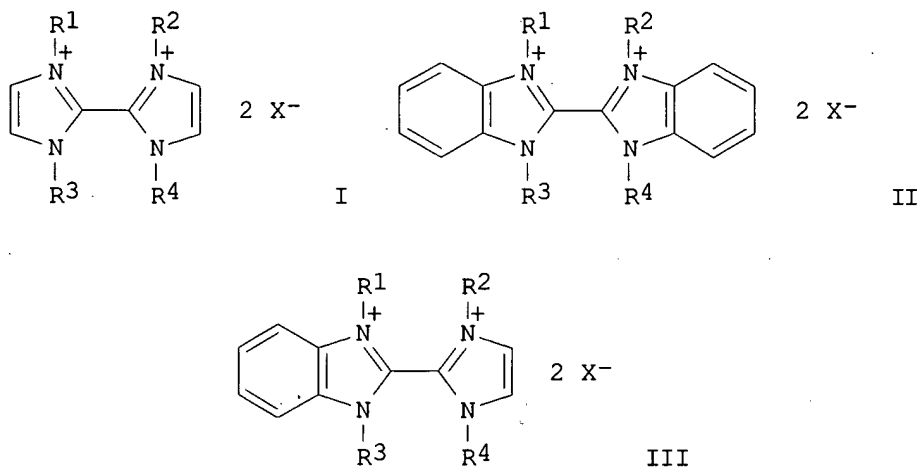
CODEN: CJCHAG; ISSN: 0008-4042

PB National Research Council of Canada

DT Journal

LA English

GI



AB Prepn. of bisannulated salts of 2,2'-biimidazole, 2-(2'-imidazolyl)benzimidazole, 2,2'-bibenzimidazole, and annulated salts of 1,1'-dimethyl-2,2'-biimidazole, 1,1'-dimethyl-1-(2'-imidazolyl)benzimidazole, and 1,1'-dimethyl-2,2'-bibenzimidazole, I, II, and III [R¹R² = (CH₂)₂, (CH₂)₃, (CH₂)₄; R¹ = R² = Me, R³R⁴ = (CH₂)₂, (CH₂)₃, (CH₂)₄, X = Br, I] is accomplished by direct alkylation of the parent azaheterocycle with excess 1,n-dihaloalkane. Discussions of the product conformations use electronic absorption spectra and NMR. The redox potentials of these salts are measured in DMF and MeCN, and become increasingly more neg. and less reversible as the systems become less planar.

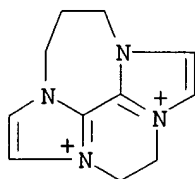
IT 120711-29-7 153652-52-9 176649-99-3

RL: PRP (Properties)

(prepn., cyclic voltammetry, and UV spectra of annulated biimidazoles, imidazolylbenzimidazoles, and bibenzimidazoles)

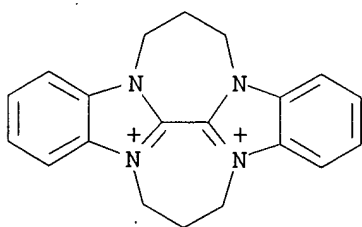
RN 120711-29-7 CAPLUS

CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[*ijkl*]-as-indacene, 3,4,8,9-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



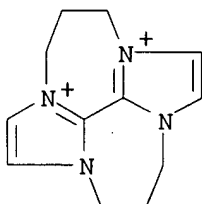
2 Br⁻

RN 153652-52-9 CAPLUS
 CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



● 2 Br⁻

RN 176649-99-3 CAPLUS
 CN 3H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene, 4,5,9,10-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



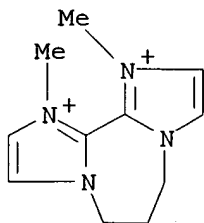
2 Br⁻

IT 188799-49-7P 188799-54-4P 188799-59-9P
 188799-63-5P 188799-67-9P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn., cyclic voltammetry, and UV spectra of annulated biimidazoles,
 imidazolylbenzimidazoles, and bibenzimidazoles)

09/868,356

RN 188799-49-7 CAPLUS

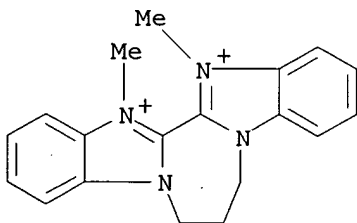
CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepinium, 6,7-dihydro-1,11-dimethyl-,
dibromide (9CI) (CA INDEX NAME)



● 2 Br⁻

RN 188799-54-4 CAPLUS

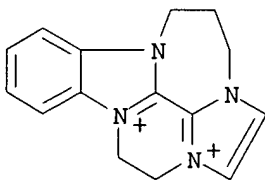
CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepinium, 7,8-dihydro-14,15-
dimethyl-, dibromide (9CI) (CA INDEX NAME)



● 2 Br⁻

RN 188799-59-9 CAPLUS

CN 9H-8b,11a-Diaza-2a,4a-diazoniaazuleno[7,8,1-lma]fluorene,
3,4,10,11-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



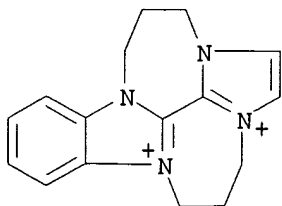
● 2 Br⁻

RN 188799-63-5 CAPLUS

CN 3H,10H-9b,12a-Diaza-2a,5a-diazoniacyclopent[ef]indeno[1,2,3-kl]heptalene,

09/868,356

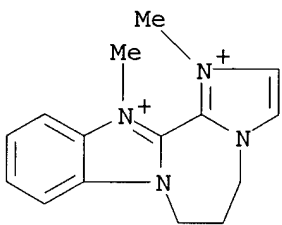
4,5,11,12-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



●2 Br⁻

RN 188799-67-9 CAPLUS

CN 5H-Imidazo[2',1':3,4][1,4]diazepino[1,2-a]benzimidazolium,
6,7-dihydro-1,13-dimethyl-, dibromide (9CI) (CA INDEX NAME)



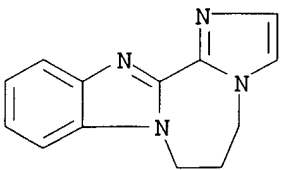
●2 Br⁻

IT 188799-45-3P

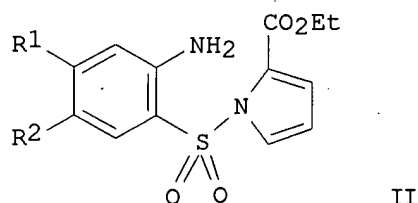
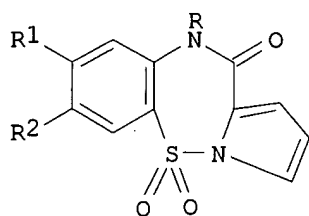
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn., cyclic voltammetry, and UV spectra of annulated biimidazoles,
imidazolylbenzimidazoles, and bibenzimidazoles)

RN 188799-45-3 CAPLUS

CN 5H-Imidazo[2',1':3,4][1,4]diazepino[1,2-a]benzimidazole, 6,7-dihydro-
(9CI) (CA INDEX NAME)



~~LS~~ ANSWER 20 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1996:432298 CAPLUS
 DN 125:195606
 TI 5H-Pyrrolo[1,2-b][1,2,5]benzothiadiazepines (PBTDs): a novel class of non-nucleoside reverse transcriptase inhibitors
 AU Artico, Marino; Silvestri, Romano; Pagnozzi, Eugenia; Stefancich, Giorgio; Massa, Silvio; Loi, Anna Giulia; Putzolu, Monica; Corrias, Simona; Spiga, Maria Grazia; La Colla, Paolo
 CS Dipartimento di Studi Farmaceutici, Universita di Roma, Rome, 00185, Italy
 SO Bioorganic & Medicinal Chemistry (1996), 4(6), 837-850
 CODEN: BMECEP; ISSN: 0968-0896
 PB Elsevier
 DT Journal
 LA English
 GI



AB With the aim of developing novel inhibitors of human immunodeficiency virus, various derivs., e.g., I (R = H, Me, Et, Pr, allyl, 2-butenyl, etc.; R1, R2 = H, Cl), related to 5H-pyrrolo[1,2-b][1,2,5]benzothiadiazepine (PBTd), were prep'd. and tested in vitro. The title tricyclic derivs. were obtained by intramol. cyclization of the open-chain intermediate aryl pyrrolyl sulfones, e.g., II, followed by N-alkylation at position 10. Among test derivs. some 10-alkyl-5H-pyrrolo[1,2b][1,2,5]benzothiadiazepin-11(10H)-one-5,5-dioxides were found to exert potent and specific activity against HIV-1. In particular, 7-chloro derivs. I (R = R1 = H, R2 = Cl; R = Me, R1 = H, R2 = Cl) showed a potency comparable to that of nevirapine. However, when the chloro atom was shifted to the 8 position, the related products were scarcely active or totally inactive. Replacement of the pyrrole with pyrrolidine led to inactive products and the redn. of SO2 to S strongly diminished the antiviral potency. PBTd derivs. active in cell cultures were also inhibitory to the recombinant HIV-1 RT in enzyme assays, thus allowing the conclusion that PBTds are a new class of non-nucleoside reverse transcriptase inhibitors (NNRTIs).

IT 153776-32-0

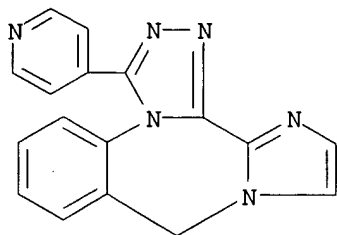
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(prepn., cytotoxicity, and anti-HIV-1 activity of pyrrolobenzothiadiazepines)

RN 153776-32-0 CAPLUS

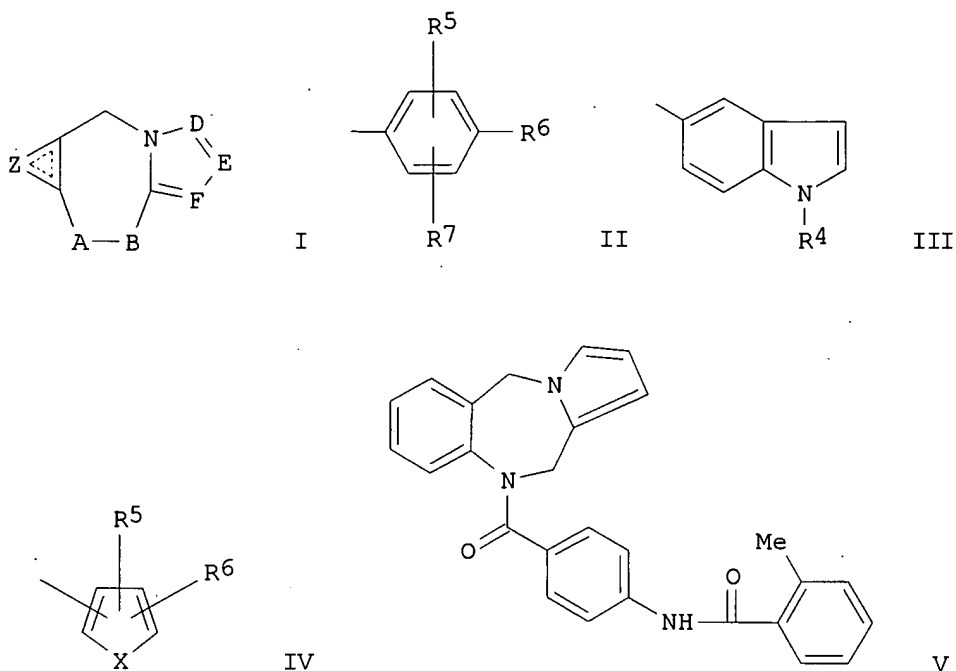
CN 9H-Imidazo[2,1-c]-1,2,4-triazolo[4,3-a][1,4]benzodiazepine, 3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

09/868,356



~~LS7~~ ANSWER 21 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1996:350579 CAPLUS
 DN 125:114720
 TI Tricyclic diazepam vasopressin antagonists and oxytocin antagonists
 IN Albright, Jay D.; Reich, Marvin F.; Sum, Fuk Wah; Delos Santos, Efren G.
 PA American Cyanamid Co., USA
 SO U.S., 116 pp., Cont.-in-part of U.S. Ser. No. 100,004, abandoned.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|------|----------|------------------|----------|
| PI | US 5516774 | A | 19960514 | US 1994-254822 | 19940613 |
| | AT 176234 | E | 19990215 | AT 1994-111039 | 19940715 |
| | ES 2129090 | T3 | 19990601 | ES 1994-111039 | 19940715 |
| | SK 280836 | B6 | 20000814 | SK 1994-881 | 19940720 |
| | CA 2128956 | AA | 19950130 | CA 1994-2128956 | 19940727 |
| | FI 9403543 | A | 19950130 | FI 1994-3543 | 19940728 |
| | NO 9402816 | A | 19950130 | NO 1994-2816 | 19940728 |
| | AU 9468777 | A1 | 19950209 | AU 1994-68777 | 19940728 |
| | AU 683660 | B2 | 19971120 | | |
| | ZA 9405603 | A | 19950309 | ZA 1994-5603 | 19940728 |
| | JP 07157486 | A2 | 19950620 | JP 1994-195857 | 19940728 |
| | HU 71495 | A2 | 19951128 | HU 1994-2219 | 19940728 |
| | RU 2126006 | C1 | 19990210 | RU 1994-27583 | 19940728 |
| | CN 1106812 | A | 19950816 | CN 1994-108769 | 19940729 |
| | CN 1039908 | B | 19980923 | | |
| | PL 178563 | B1 | 20000531 | PL 1994-304498 | 19940729 |
| | TW 397834 | B | 20000711 | TW 1994-83108600 | 19940916 |
| | US 5624923 | A | 19970429 | US 1995-468737 | 19950606 |
| | US 5733905 | A | 19980331 | US 1996-646582 | 19960508 |
| | US 5736540 | A | 19980407 | US 1996-646841 | 19960508 |
| | US 5889001 | A | 19990330 | US 1997-874835 | 19970613 |
| | US 5854237 | A | 19981229 | US 1997-877314 | 19970617 |
| | US 5843944 | A | 19981201 | US 1997-893636 | 19970711 |
| | US 5968930 | A | 19991019 | US 1997-999830 | 19971003 |
| | CN 1205335 | A | 19990120 | CN 1998-103834 | 19980210 |
| | CN 1056374 | B | 20000913 | | |
| | HK 1011363 | A1 | 20000505 | HK 1998-112375 | 19981127 |
| | US 5968937 | A | 19991019 | US 1998-207522 | 19981208 |
| | LV 12497 | B | 20000920 | LV 2000-13 | 20000127 |
| | FI 2001001206 | A | 20010607 | FI 2001-1206 | 20010607 |
| | FI 2001001207 | A | 20010607 | FI 2001-1207 | 20010607 |
| PRAI | US 1993-100004 | B2 | 19930729 | | |
| | US 1994-254822 | A3 | 19940613 | | |
| | US 1995-468737 | A2 | 19950606 | | |
| | US 1996-646542 | B1 | 19960508 | | |
| | US 1996-646582 | A1 | 19960508 | | |
| | US 1996-646653 | B1 | 19960508 | | |
| | US 1997-999830 | A3 | 19971003 | | |
| OS | MARPAT 125:114720 | | | | |
| GI | | | | | |



AB Tricyclic diazepines of the formula I wherein: A-B is (CH₂)NR₃ or NR₃CH₂; the fused Z ring represents a fused Ph or fused Ph optionally substituted by one or two substituents selected from (C1-C3) lower alkyl, halogen, amino, (C1-C3) lower alkoxy, or (C1-C3) lower alkylamino; the fused DEF ring is a five-membered arom. (unsatd.) fused nitrogen-contg. heterocyclic ring wherein D, E, and F are carbon and wherein the carbon atoms may be optionally substituted by a substituent selected from, e.g., halogen, (C1-C3) lower alkyl, hydroxy, COCl, COCF₃; R₃ = COAr, wherein Ar is selected from II-IV; X = O, S, NH, NMe, NAc; R₄ = e.g., H, (C1-C3) lower alkyl; R₅ = e.g., H, (C1-C3) lower alkyl; R₆ = e.g., amido, aminocarbonyl, ureido; R₇ = e.g., H, (C1-C3) lower alkyl; have vasopressin and oxytocin antagonist activity. Thus, e.g., amidation of 4-[(2-methylbenzoyl)amino]benzoyl chloride with 10,11-dihydro-5H-pyrrolo[2,1-c][1,4]benzodiazepine afforded benzamide V which at 1-10 mg/kg exhibited vasopressin V2 antagonist activity in conscious hydrated rats (increased urine vol. and decreased osmolality relative to control), vasopressin V1 antagonist activity (e.g., 70% inhibition of vasopressin vasopressor response in conscious rats at 3 mg/kg i.v.), and 90% inhibition of oxytocin receptor binding at 10 .mu.M with IC₅₀ = 0.36 .mu.M. V exhibited binding to rat hepatic V1 receptors and rat kidney medullary V2 receptors with IC₅₀ = 0.038 and 0.004 .mu.M, resp.

IT 179063-03-7P 179063-04-8P 179063-05-9P

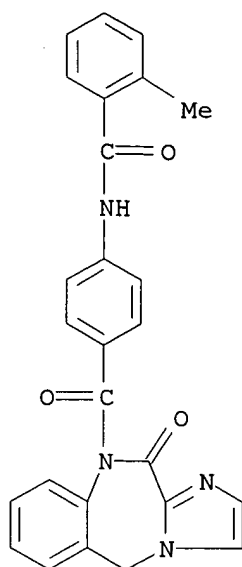
179063-06-0P 179063-10-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(tricyclic diazepine vasopressin antagonists and oxytocin antagonists)

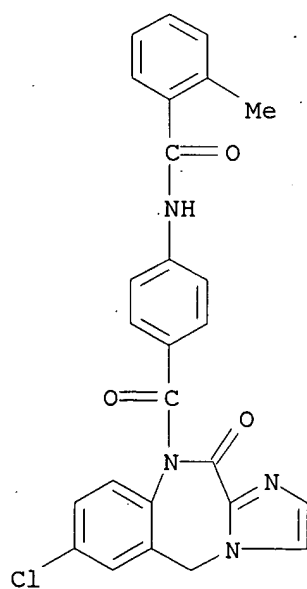
RN 179063-03-7 CAPLUS

CN Benzamide, 2-methyl-N-[4-[(11-oxo-5H-imidazo[2,1-a][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



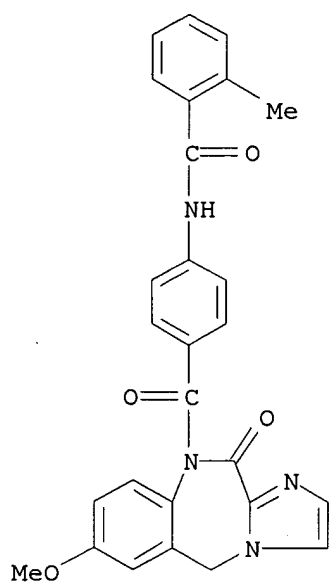
RN 179063-04-8 CAPLUS

CN Benzamide, N-[4-[(7-chloro-11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



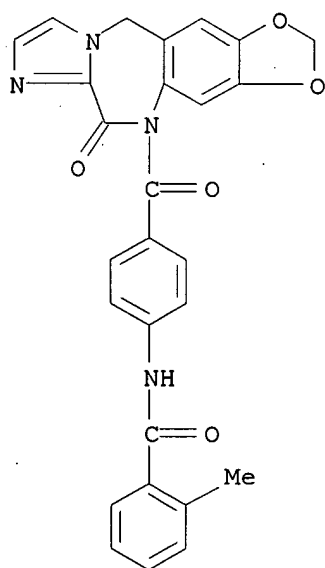
RN 179063-05-9 CAPLUS

CN Benzamide, N-[4-[(7-methoxy-11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



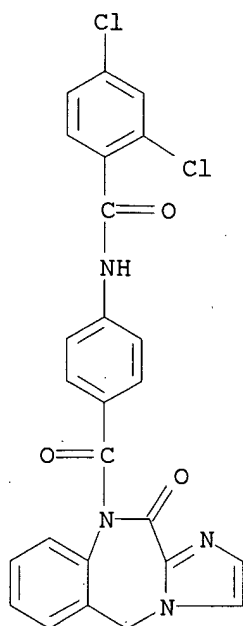
RN 179063-06-0 CAPLUS

CN Benzamide, 2-methyl-N-[4-[(6-oxo-6H-1,3-dioxolo[4,5-h]imidazo[2,1-c][1,4]benzodiazepin-5(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



RN 179063-10-6 CAPLUS

CN Benzamide, 2,4-dichloro-N-[4-[(11-oxo-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]- (9CI) (CA INDEX NAME)



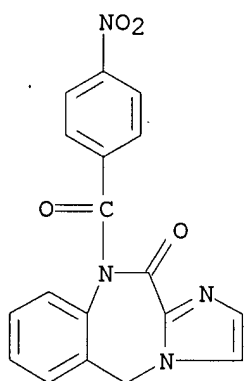
IT 179063-15-1P 179063-16-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(tricyclic diazepine vasopressin antagonists and oxytocin antagonists)

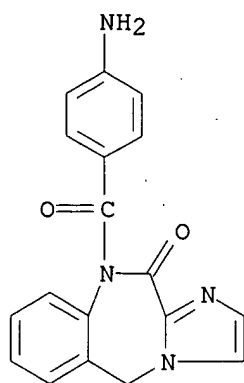
RN 179063-15-1 CAPLUS

CN 11H-Imidazo[2,1-c][1,4]benzodiazepin-11-one, 5,10-dihydro-10-(4-nitrobenzoyl)- (9CI) (CA INDEX NAME)



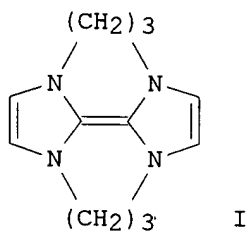
RN 179063-16-2 CAPLUS

CN 11H-Imidazo[2,1-c][1,4]benzodiazepin-11-one, 10-(4-aminobenzoyl)-5,10-dihydro- (9CI) (CA INDEX NAME)

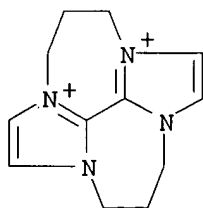


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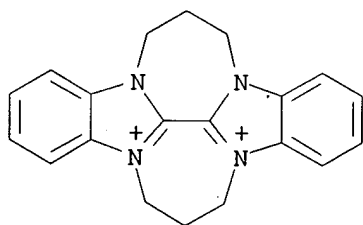
~~LE~~ ANSWER 22 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~IN~~ 1996:319160 CAPLUS
DN 125:86606
TI A stable tetraazafulvalene
AU Taton, T. Andrew; Chen, Peter
CS Laboratorium Organische Chemie, Eidgenossischen Technischen Hochschule
Universitaetstrasse, Zurich, CH-8092, Switz.
SO Angewandte Chemie, International Edition in English (1996), 35(9),
1011-1013
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI



AB Tetraazafulvalene I was prepd. by two routes and its crystal structure
dtd.
IT **162477-59-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and crystal structure of tetraazafulvalene)
RN 162477-59-0 CAPLUS
CN 3H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene,
4,5,9,10-tetrahydro- (9CI) (CA INDEX NAME)



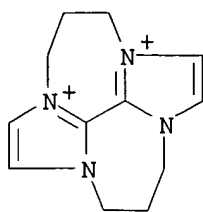
~~127~~ ANSWER 23 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1996:213415 CAPLUS
 DN 124:343249
 TI An aza-analog of TTF: 1,1';3,3'-bistrimethylene-2,2'-diimidazolinylidene
 AU Shi, Zhiqiang; Gouille, Véronique; Thummel, Randolph P.
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SO Tetrahedron Letters (1996), 37(14), 2357-60
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 AB Bulk electrolysis of 1,1';3,3'-bistrimethylene-2,2'-biimidazolium dibromide at -1.6 V in acetonitrile provides the air sensitive 1,1';3,3'-bistrimethylene-2,2'-diimidazolinylidene which was characterized by ¹H and ¹³C NMR. The corresponding dinaphtho-fused species, prepd. by deprotonation of a bis-trimethylene bridged bis-naphth[2,3]imidazolium dibromide, reacts readily with air to form a syn-ureaphane.
 IT **153652-52-9**
 RL: PRP (Properties)
 (prepn. of bistrimethylenediimidazolinylidene)
 RN 153652-52-9 CAPLUS
 CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



●2 Br⁻

IT **176649-99-3**
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of bistrimethylenediimidazolinylidene)
 RN 176649-99-3 CAPLUS
 CN 3H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene, 4,5,9,10-tetrahydro-, dibromide (9CI) (CA INDEX NAME)

09/868,356



●2 Br⁻

~~127~~ ANSWER 24 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1995:903092 CAPLUS

DN 123:305145

TI 4,4'-Bis(2-picolinimino)-2,2'-bibenzimidazoles: A New Class of Dinucleating Ligands Which Allow for a Tuning of the Metal-Metal Distance. Structures and Properties of a Dicopper(II) Complex and of Two Oxygenation Products of a Dicopper(I) Complex; a Tentative Coordination Chemical Modeling of Hemocyanin

AU Muller, Edgar; Bernardinelli, Gerald; Reedijk, Jan

CS Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.

SO Inorganic Chemistry (1995), 34(24), 5979-88

CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

AB 4,4'-Bis(2-picolinimino)-2,2'-bibenzimidazole derivs. (L), derived from 1,1'-disubstituted 4,4'-diamino-2,2'-bibenzimidazoles and 2-pyridinecarboxaldehyde, were developed as models for type 3 sites of the copper proteins hemocyanin and tyrosinase. These hollow, ditopic ligands can hold two metal ions face to face at distances of 3.15 .ANG. or larger. The metal-metal distance can be restricted (tuned) to a given value via a corresponding polymethylene bridge in the ligand's backbone. [CuII2(L)(DMF)3(H2O)2](F3CSO3)4 [L = 1,1',5,5',6,6'-hexamethyl-4,4'-bis(2-picolinimino)-2,2'-bibenzimidazole] (space group P.hivin.1, a 14.811(21), b 15.358(26), c 16.209(9) .ANG., .alpha. 95.57(9), .beta. 107.56(9), .gamma. 110.35(13).degree., Z = 2) presents an open conformation with discrete (4 + 2) copper coordination environments, where two DMF mols. occupy the 4th positions of the equatorial CuN3O squares (.ltbbrac.Cu-N.rtbbrac. = 2.02 .ANG., .ltbbrac.Cu-O.rtbbrac. = 1.95 .ANG.). Two water mols., a DMF and one of the triflate anions, are coordinated to the four axial positions (Cu-O of 2.28-2.74 .ANG.). The two halves of the ligand are rotated out of the cis-coplanar conformation by 115.7.degree., resulting in a relatively long Cu.cntdot..cntdot..cntdot.Cu distance of 6.16 .ANG.. In acetonitrile, the complex shows two irreversible Cu(II)/Cu(I) redox potentials at 0.60 and 0.30 V (normal H electrode). Two oxygenation products of the dicopper(I) complex of the restricted ligand 1,1'-trimethylene-5,5',6,6'-tetramethyl-4,4'-bis(2-picolinimino)-2,2'-bibenzimidazole (L3), which best approaches the geometry of a type 3 site, were isolated in the cryst. state. The 1st one, [CuII4(H2(L3)O22-)-2](ClO4)4 (orthorhombic: space group Ccca, a 16.171(3), b 19.760(4), c 22.168(5) .ANG., Z = 4), is a tetranuclear copper(II) cluster, best described as a sym. Cu4O4 eight membered ring (Cu.cntdot..cntdot..cntdot.Cu distances of 3.05, 3.50, and 6.30 .ANG.), attached to two L3 mols., with the four oxy anions covalently linked to the azomethine carbons (forming the L3 deriv. H2(L3)O22-). The 2nd oxygenation product, [CuI2(L3')2](ClO4)2 (monoclinic: space group C2/c, a 23.500(3), b 12.569(5), c 19.926(8) .ANG., .beta. 106.71(2).degree., Z = 4), is a dinuclear copper(I) complex of L3', a degrdn. product of L3, carrying a free amino group on one side. The copper(II) ions are in a bis(diimine) type, distorted tetrahedral environment (dihedral angle 79.1.degree.), with a Cu.cntdot..cntdot..cntdot.Cu distance of 4.59 .ANG.. About 25% of the ligand L3' appears to be oxidized at the free amino group to the corresponding quinonimine, as deduced from the x-ray structure detn.

IT 169699-42-7P 169699-45-0P 169699-48-3P

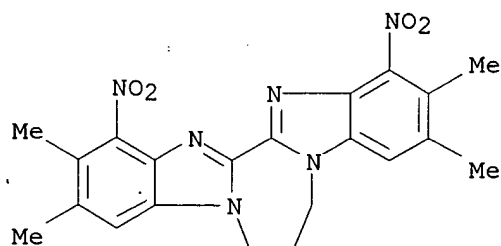
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepn. of copper bis(picolinimino)bibenzimidazole deriv. dinuclear

complexes as hemocyanin models).

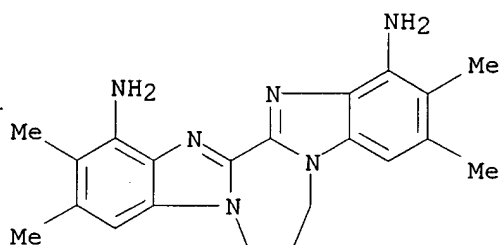
RN 169699-42-7 CAPLUS

CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine, 7,8-dihydro-2,3,11,12-tetramethyl-1,13-dinitro- (9CI) (CA INDEX NAME)



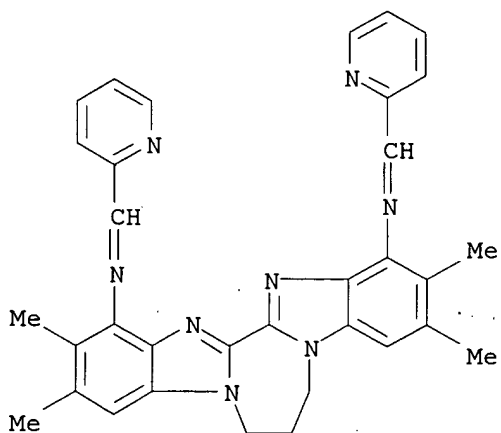
RN 169699-45-0 CAPLUS

CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine-1,13-diamine, 7,8-dihydro-2,3,11,12-tetramethyl- (9CI) (CA INDEX NAME)



RN 169699-48-3 CAPLUS

CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine-1,13-diamine, 7,8-dihydro-2,3,11,12-tetramethyl-N,N'-bis(2-pyridinylmethylene)- (9CI) (CA INDEX NAME)



IT 169699-38-1P 169699-40-5DP, solid soln. with partially oxidized analogous complex 169699-53-0DP, solid soln. with

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unoxidized analogous complex

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of copper bis(picolinimino)bibenzimidazole deriv. dinuclear complexes as hemocyanin models)

RN 169699-38-1 CAPLUS

CN Copper(4+), bis[.mu.3-[[.alpha.,.alpha.'-[(7,8-dihydro-2,3,11,12-tetramethyl-6H-bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine-1,13-diyl)diimino]bis[2-pyridinemethanolato]](2-))]tetra-, stereoisomer, tetraperchlorate (9CI) (CA INDEX NAME)

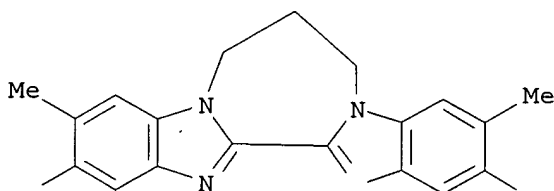
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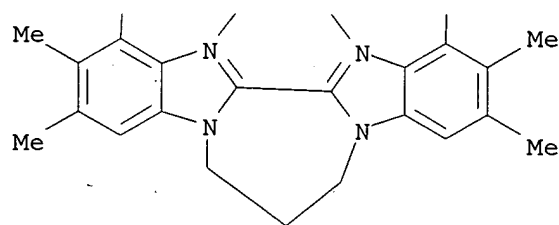
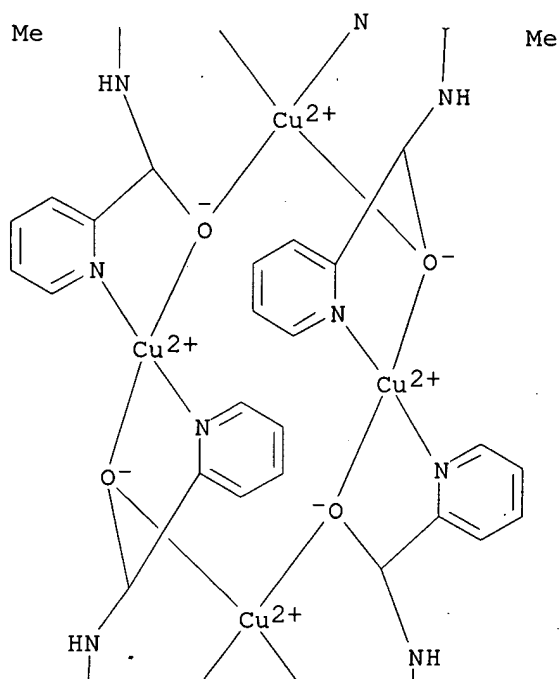
CRN 169699-37-0

CMF C66 H64 Cu4 N16 O4

CCI CCS

PAGE 1-A

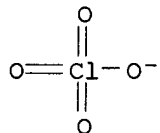




CM 2

CRN 14797-73-0

CMF Cl O4



RN 169699-40-5 CAPLUS

CN Copper(2+), bis[.mu.-[7,8-dihydro-2,3,11,12-tetramethyl-N-(2-pyridinylmethylene)-6H-bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine-1,13-

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diamine-N1,N1':N14,N15]]di-, diperchlorate (9CI) (CA INDEX NAME)

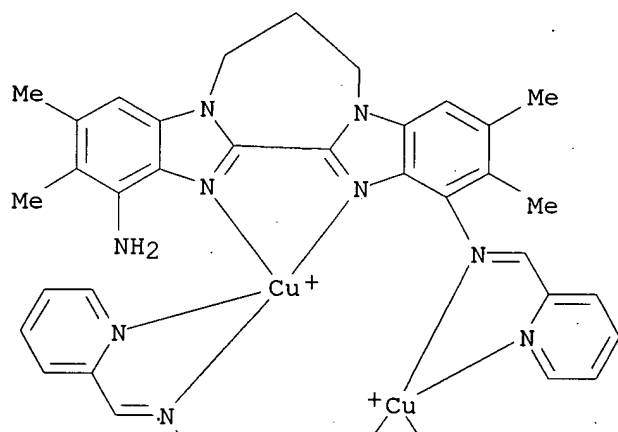
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CRN 169699-39-2

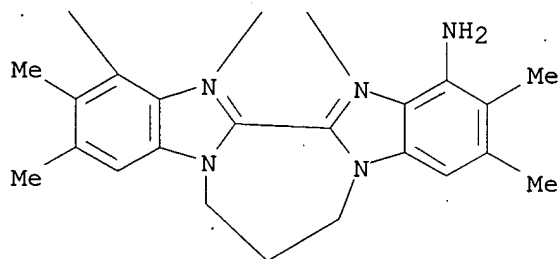
CMF C54 H54 Cu2 N14

CCI CCS

PAGE 1-A



PAGE 2-A

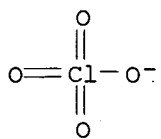


CM 2

CRN 14797-73-0

CMF C1 O4

09/868,356

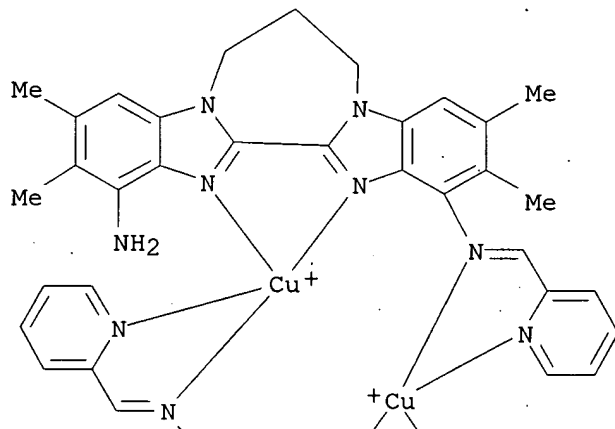


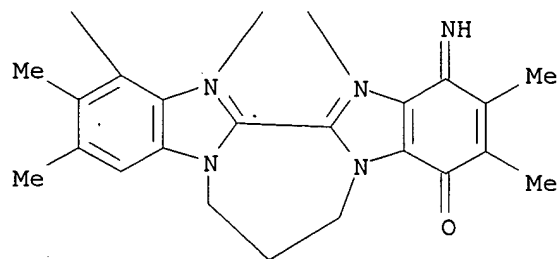
RN 169699-53-0 CAPLUS
CN Copper(2+), bis[.mu.-[7,8-dihydro-1-imino-2,3,11,12-tetramethyl-13-[(2-pyridinylmethylene)amino]-6H-bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepin-4(1H)-one-N13,N13':N14,N15]]di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 169699-52-9
CMF C54 H52 Cu2 N14 O
CCI CCS

PAGE 1-A

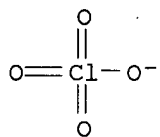




CM 2

CRN 14797-73-0

CMF Cl O4



~~127~~ ANSWER 25 OF 46 CAPLUS COPYRIGHT 2003 ACS

IN 1995:810397 CAPLUS

DN 123:228225

TI Preparation of tricyclic diazepines and related compounds as vasopressin and oxytocin antagonists.

IN Albright, Jay D.; Reich, Marvin F.; Sum, Fuk-Wah; Delos Santos, Efren Guillermo

PA American Cyanamid Co., USA

SO Eur. Pat. Appl., 256 pp.

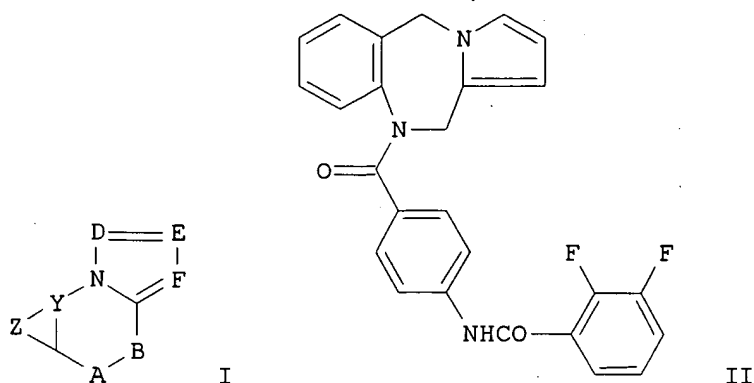
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 4

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|------------------|----------|
| PI | EP 636625 | A2 | 19950201 | EP 1994-111039 | 19940715 |
| | EP 636625 | A3 | 19950517 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| | AT 176234 | E | 19990215 | AT 1994-111039 | 19940715 |
| | ES 2129090 | T3 | 19990601 | ES 1994-111039 | 19940715 |
| | SK 280836 | B6 | 20000814 | SK 1994-881 | 19940720 |
| | CA 2128956 | AA | 19950130 | CA 1994-2128956 | 19940727 |
| | FI 9403543 | A | 19950130 | FI 1994-3543 | 19940728 |
| | NO 9402816 | A | 19950130 | NO 1994-2816 | 19940728 |
| | AU 9468777 | A1 | 19950209 | AU 1994-68777 | 19940728 |
| | AU 683660 | B2 | 19971120 | | |
| | ZA 9405603 | A | 19950309 | ZA 1994-5603 | 19940728 |
| | JP 07157486 | A2 | 19950620 | JP 1994-195857 | 19940728 |
| | HU 71495 | A2 | 19951128 | HU 1994-2219 | 19940728 |
| | RU 2126006 | C1 | 19990210 | RU 1994-27583 | 19940728 |
| | CN 1106812 | A | 19950816 | CN 1994-108769 | 19940729 |
| | CN 1039908 | B | 19980923 | | |
| | PL 178563 | B1 | 20000531 | PL 1994-304498 | 19940729 |
| | TW 397834 | B | 20000711 | TW 1994-83108600 | 19940916 |
| | CN 1205335 | A | 19990120 | CN 1998-103834 | 19980210 |
| | CN 1056374 | B | 20000913 | | |
| | HK 1011363 | A1 | 20000505 | HK 1998-112375 | 19981127 |
| | LV 12497 | B | 20000920 | LV 2000-13 | 20000127 |
| | FI 2001001206 | A | 20010607 | FI 2001-1206 | 20010607 |
| | FI 2001001207 | A | 20010607 | FI 2001-1207 | 20010607 |
| PRAI | US 1993-100004 | A | 19930729 | | |
| OS | CASREACT 123:228225; MARPAT 123:228225 | | | | |
| GI | | | | | |



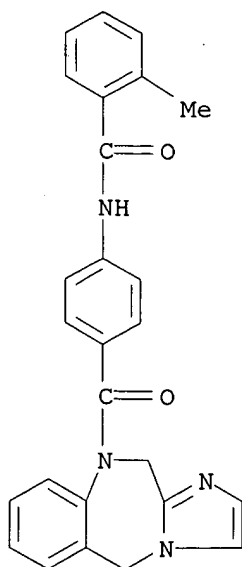
AB Title compds. [I; Y = (CH₂)_n, RCH, CO; n = 0-2; R = C1-3 alkyl; AB = (CH₂)_mNR₃; R₃ = COAr; Ar = (substituted) indolyl, acylaminophenyl, -furyl, -thienyl, -pyrrolyl, etc.; m = 0-3, with provisos; Z = atoms to form a (substituted) fused Ph, (unsatd.) heterocyclyl; D, E, F = N or C which may be substituted], were prepd. Thus, 2,3-difluorobenzoyl chloride in CH₂Cl₂ was treated with Et₃N and then with 10,11-dihydro-(4-aminobenzoyl)-5H-pyrrolo[2,1-c][1,4]benzodiazepine (prepn. given) to give title compd. (II). II showed IC₅₀ = 0.097 .mu.M and 0.029 .mu.M in binding assays for vasopressin V₁ and V₂ receptors, resp.

IT **168078-73-7P 168078-76-0P 168078-77-1P**
168078-78-2P 168080-00-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of tricyclic diazepines and related compds. as vasopressin and oxytocin antagonists)

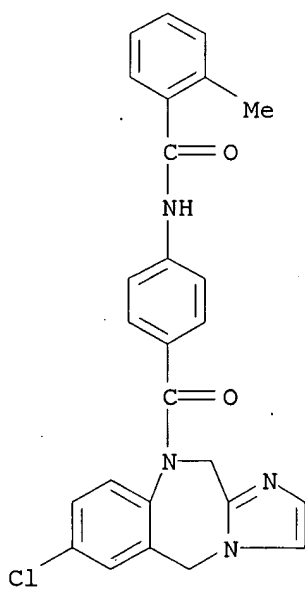
RN 168078-73-7 CAPLUS

CN Benzamide, N-[4-(5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)phenyl]-2-methyl- (9CI) (CA INDEX NAME)



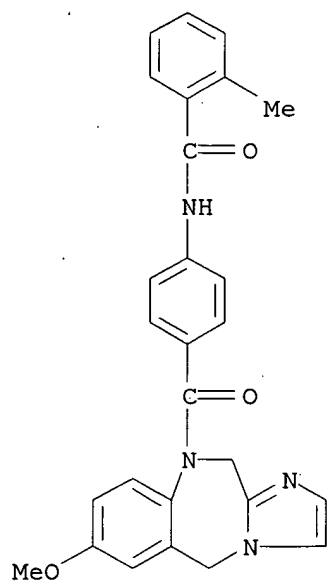
RN 168078-76-0 CAPLUS

CN Benzamide, N-[4-[(7-chloro-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



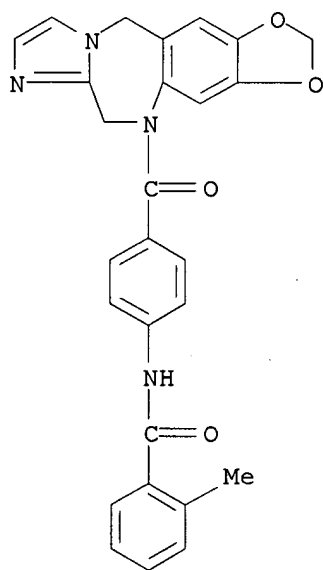
RN 168078-77-1 CAPLUS

CN Benzamide, N-[4-[(7-methoxy-5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-yl)carbonyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



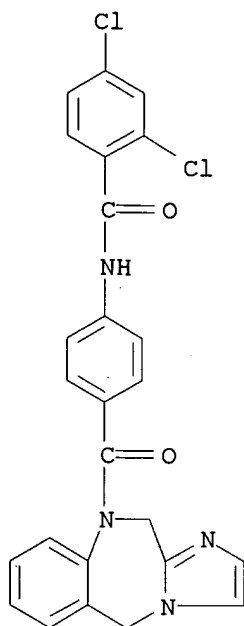
RN 168078-78-2 CAPLUS

CN Benzamide, N-[4-(6H-1,3-dioxolo[4,5-h]imidazo[2,1-c][1,4]benzodiazepin-5(11H)-ylcarbonyl)phenyl]-2-methyl- (9CI) (CA INDEX NAME)



RN 168080-00-0 CAPLUS

CN Benzamide, 2,4-dichloro-N-[4-(5H-imidazo[2,1-c][1,4]benzodiazepin-10(11H)-ylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)



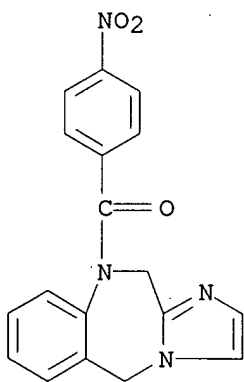
IT 168078-74-8P 168078-75-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of tricyclic diazepines and related compds. as vasopressin and oxytocin antagonists)

RN 168078-74-8 CAPLUS

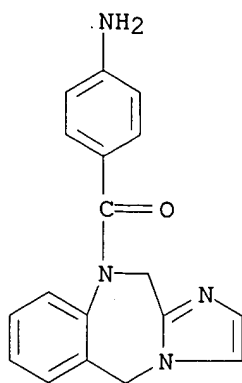
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-10-(4-nitrobenzoyl)-(9CI) (CA INDEX NAME)



RN 168078-75-9 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10-(4-aminobenzoyl)-10,11-dihydro-(9CI) (CA INDEX NAME)

09/868,356



127 ANSWER 26 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1995:792607 CAPLUS

DN 123:198837

TI Preparation of tricyclic benzodiazepinone inhibitors of the GPIIb/IIIa fibrinogen receptor which block blood platelet aggregation

IN Blackburn, Brent K.; Robarge, Kirk; Somers, Todd C.

PA Genentech, Inc., USA

SO PCT Int. Appl., 355 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9504057 | A1 | 19950209 | WO 1994-US7989 | 19940715 |
| | W: CA, JP, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | US 5493020 | A | 19960220 | US 1993-99019 | 19930729 |
| | EP 708775 | A1 | 19960501 | EP 1994-923512 | 19940715 |
| | EP 708775 | B1 | 19970528 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| | JP 09501158 | T2 | 19970204 | JP 1994-505853 | 19940715 |
| | AT 153665 | E | 19970615 | AT 1994-923512 | 19940715 |
| | US 5705890 | A | 19980106 | US 1994-313069 | 19940926 |
| PRAI | US 1993-99019 | | 19930729 | | |
| | WO 1994-US7989 | | 19940715 | | |
| OS | MARPAT 123:198837 | | | | |
| GI | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; A1 = (un)substituted CH₂, (un)substituted CH, N, (un)substituted NH; A2 = (un)substituted CH₂, N, SO₂, SO, S, O, C:O, etc.; L = (un)substituted alkylene, (un)substituted cycloalkylene, arylene, etc.; Q = (un)substituted NH₂, (un)substituted amidino, etc.; R₁, R₂ = H, halogen, CN, CO₂H, aminocarbonyl, carboxamido, etc.; R₁₈-R₂₁ = H, alkyl, halogen, alkoxy, CN, CO₂H, OH, etc.; R₂₂ = HO, alkoxy, alkenoxy, aryloxy, etc.] [II; B1 = (un)substituted CH, (un)substituted CH₂, N, (un)substituted NH, C:O; B2 = (un)substituted CH, (un)substituted CH₂, (un)substituted NH, SO₂, SO, S, O, C:O; B3 = (un)substituted CH, (un)substituted CH₂, C:O], which potentially inhibit fibrinogen binding to the GPIIb/IIIa receptor and are useful for the treatment of diseases (no data) in which blocking platelet aggregation is indicated, are prepd. Thus, benzodiazepinone, III, was prepd. and demonstrated IC₅₀ 0.009 .mu.M for Fg/GPIIb/IIIa and 0.133 for platelet aggregation inhibition (citrate).

IT 167854-23-1P 167854-25-3P 167854-27-5P

167854-29-7P 167854-31-1P 167854-65-1P

167854-67-3P 167854-69-5P 167854-70-8P

167854-72-0P 167854-74-2P 167854-76-4P

167854-78-6P 167854-80-0P 167854-82-2P

167854-84-4P 167854-86-6P 167854-88-8P

167854-90-2P 167854-92-4P 167854-94-6P

167854-96-8P 167854-98-0P 167855-00-7P

RL: PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

09/868,356

(claimed compd.; prepn. of tricyclic benzodiazepinone inhibitors of the GPIIb/IIIa fibrinogen receptor which block blood platelet aggregation)

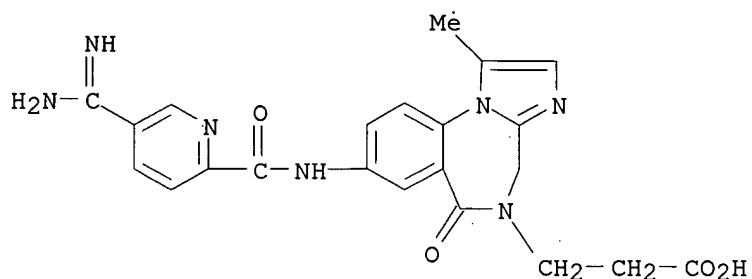
RN 167854-23-1 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[[5-(aminoiminomethyl)-2-pyridinyl]carbonyl]amino]-1-methyl-6-oxo-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-22-0

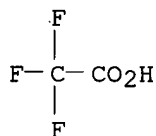
CMF C22 H21 N7 O4



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-25-3 CAPLUS

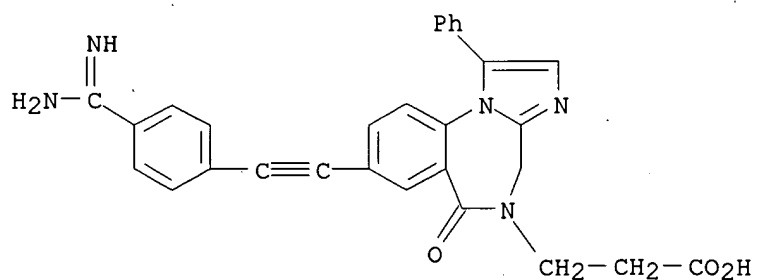
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[[4-(aminoiminomethyl)phenyl]ethynyl]-6-oxo-1-phenyl-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

CRN 167854-24-2

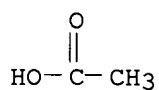
CMF C29 H23 N5 O3

09/868,356



CM 2

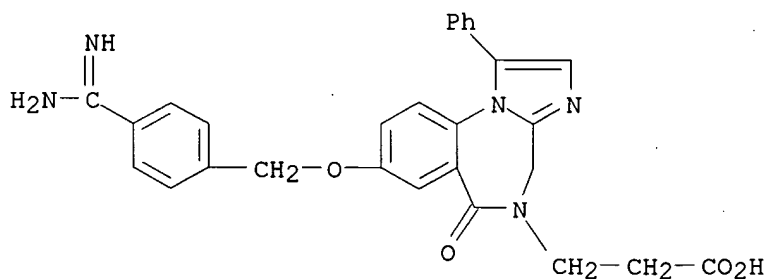
CRN 64-19-7
CMF C2 H4 O2



RN 167854-27-5 CAPLUS
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8-[[4-(aminoiminomethyl)phenyl]methoxy]-6-oxo-1-phenyl-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

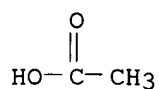
CRN 167854-26-4
CMF C28 H25 N5 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

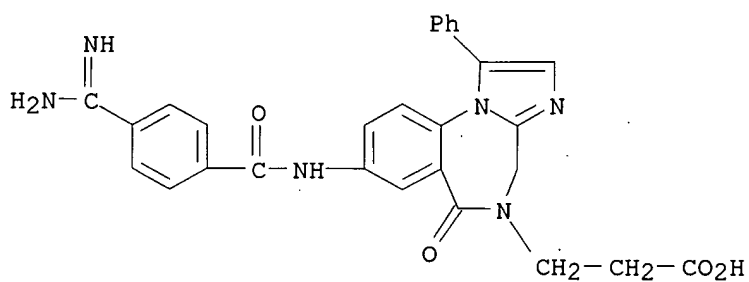
09/868,356



RN 167854-29-7 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-6-oxo-1-phenyl-, monoacetate (9CI)
(CA INDEX NAME)

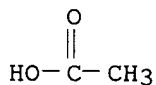
CM 1

CRN 167854-28-6
CMF C28 H24 N6 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

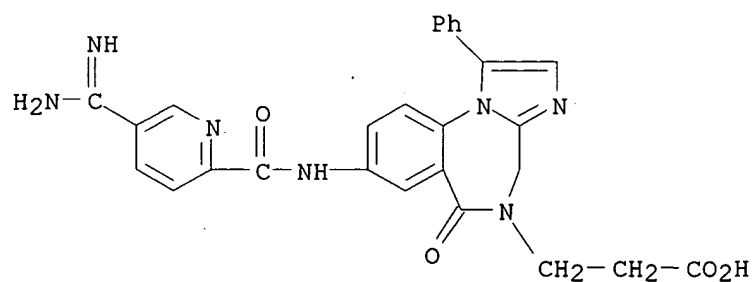


RN 167854-31-1 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[[5-(aminoiminomethyl)-2-pyridinyl]carbonyl]amino]-6-oxo-1-phenyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

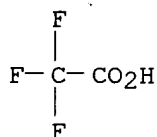
CRN 167854-30-0
CMF C27 H23 N7 O4

09/868,356



CM 2

CRN 76-05-1
CMF C2 H F3 O2

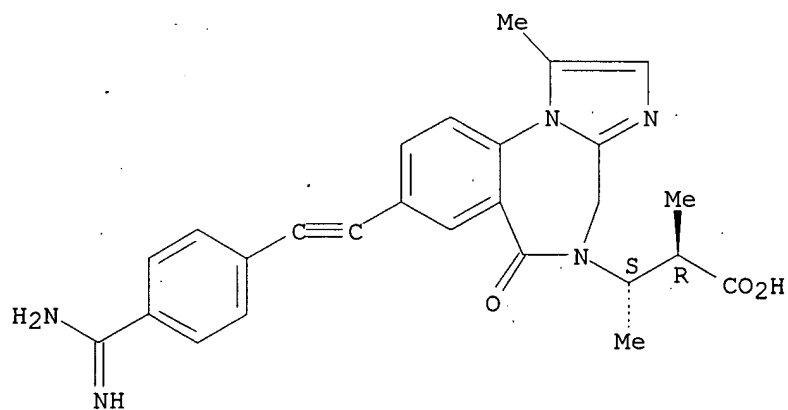


RN 167854-65-1 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-oxo-,
[S-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-64-0
CMF C26 H25 N5 O3

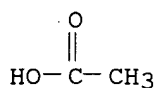
Absolute stereochemistry.



CM 2

09/868,356

CRN 64-19-7
CMF C2 H4 O2

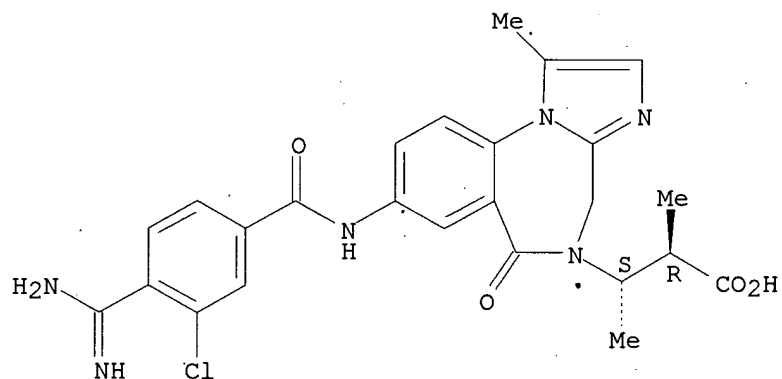


RN 167854-67-3 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorobenzoyl]amino]-.alpha.,.beta.,1-trimethyl-
6-oxo-, [S-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

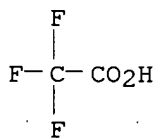
CRN 167854-66-2
CMF C25 H25 Cl N6 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 167854-69-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorobenzoyl]amino]-.alpha.,.beta.,1-trimethyl-
6-oxo-, [S-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

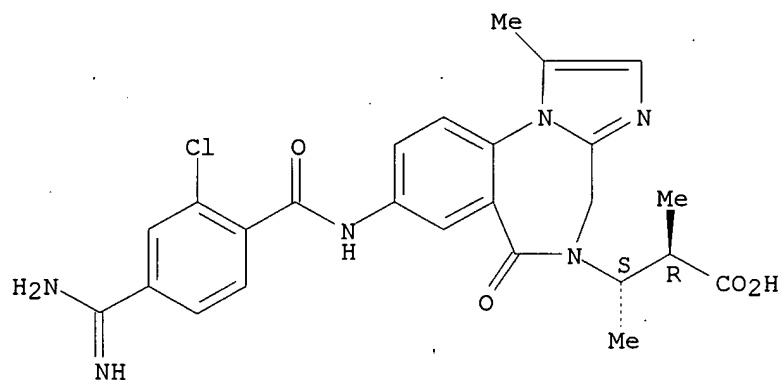
CM 1

CRN 167854-68-4

09/868,356

CMF C25 H25 Cl N6 O4

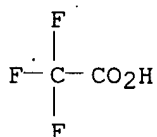
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-70-8 CAPLUS

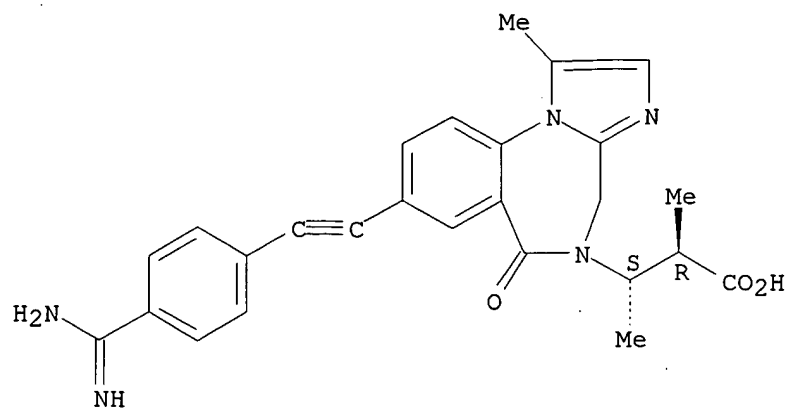
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-oxo-,
[S-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-64-0

CMF C26 H25 N5 O3

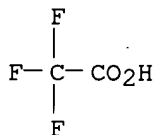
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-72-0 CAPLUS

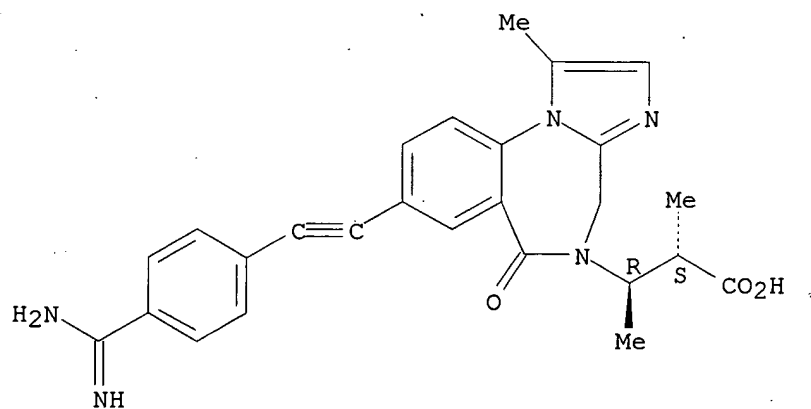
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-oxo-,
[R-(R*,S*)]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-71-9

CMF C26 H25 N5 O3

Absolute stereochemistry.

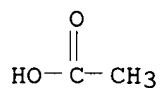


09/868,356

CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 167854-74-2 CAPLUS

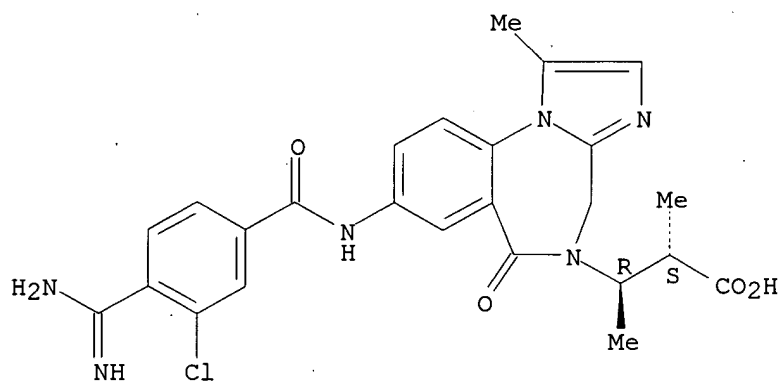
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorobenzoyl]amino]-.alpha.,.beta.,1-trimethyl-
6-oxo-, [R-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-73-1

CMF C25 H25 Cl N6 O4

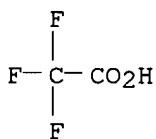
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-76-4 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorobenzoyl]amino]-.alpha.,.beta.,1-trimethyl-
6-oxo-, [R-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

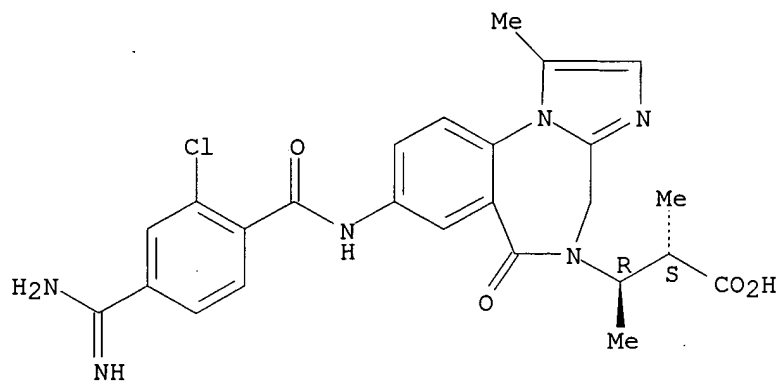
09/868,356

CM 1

CRN 167854-75-3

CMF C25 H25 Cl N6 O4

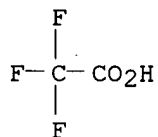
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-78-6 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,.beta.,1-trimethyl-6-
oxo-, [R-(R*,S*)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

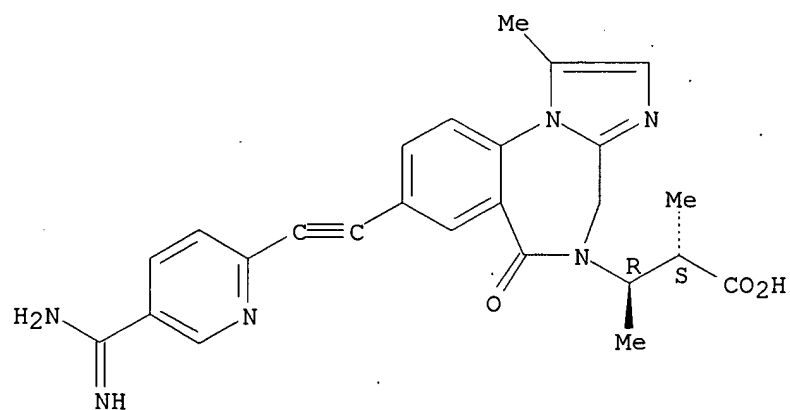
CM 1

CRN 167854-77-5

CMF C25 H24 N6 O3

Absolute stereochemistry.

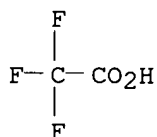
09/868,356



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-80-0 'CAPLUS

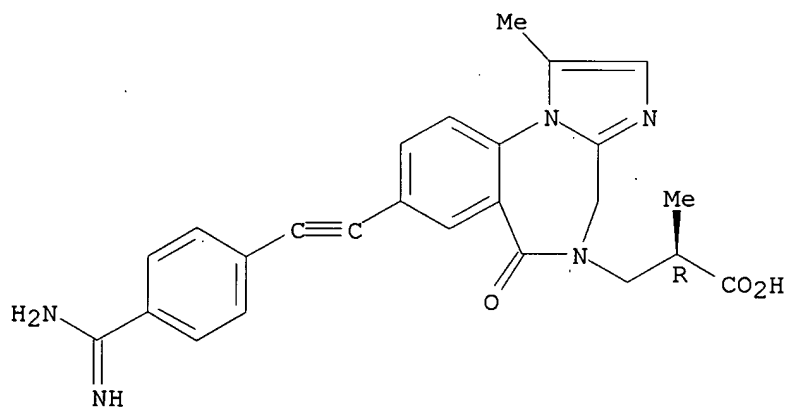
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-, (R)-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-79-7

CMF C25 H23 N5 O3

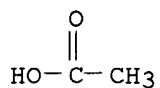
Absolute stereochemistry.



09/868,356

CM 2

CRN 64-19-7
CMF C2 H4 O2

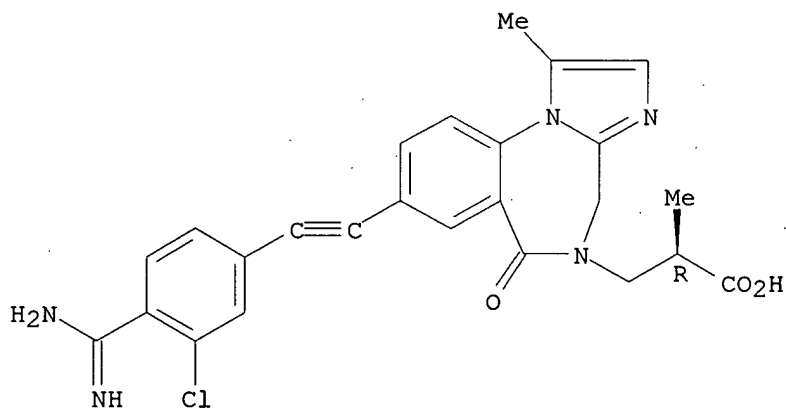


RN 167854-82-2 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-
, (R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

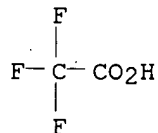
CRN 167854-81-1
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 167854-84-4 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-

09/868,356

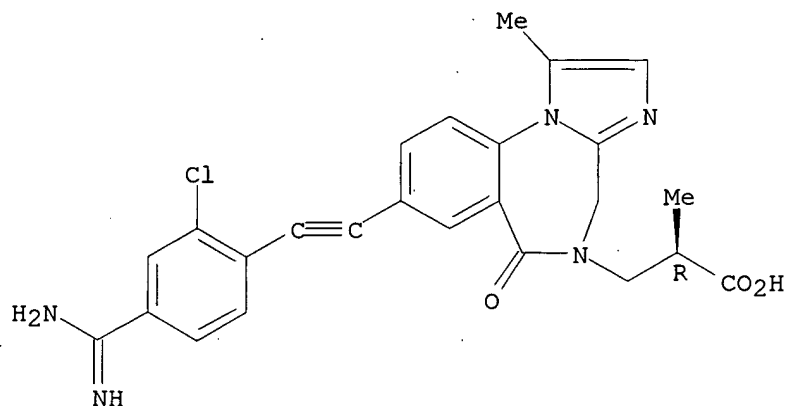
, (R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-83-3

CMF C25 H22 Cl N5 O3

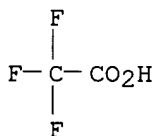
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-86-6 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-,
(R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

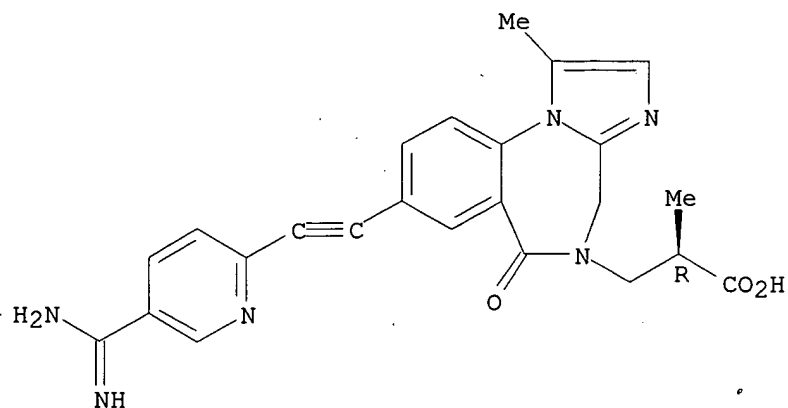
CM 1

CRN 167854-85-5

CMF C24 H22 N6 O3

Absolute stereochemistry.

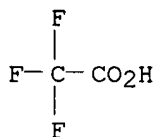
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-88-8 CAPLUS

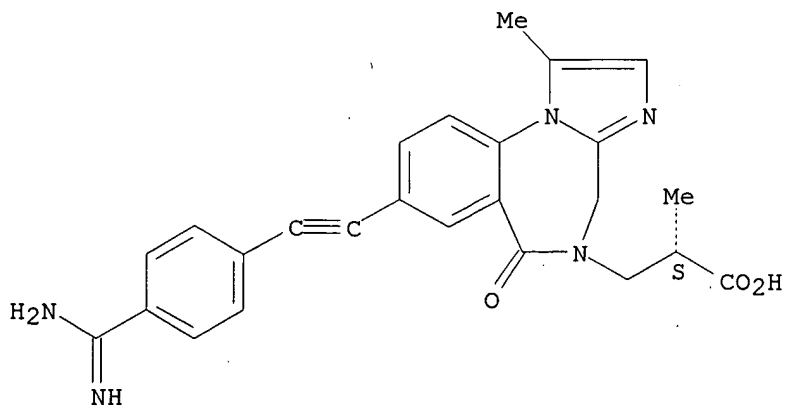
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-, (S)-,
monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167854-87-7

CMF C25 H23 N5 O3

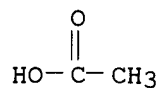
Absolute stereochemistry.



09/868,356

CM 2

CRN 64-19-7
CMF C2 H4 O2

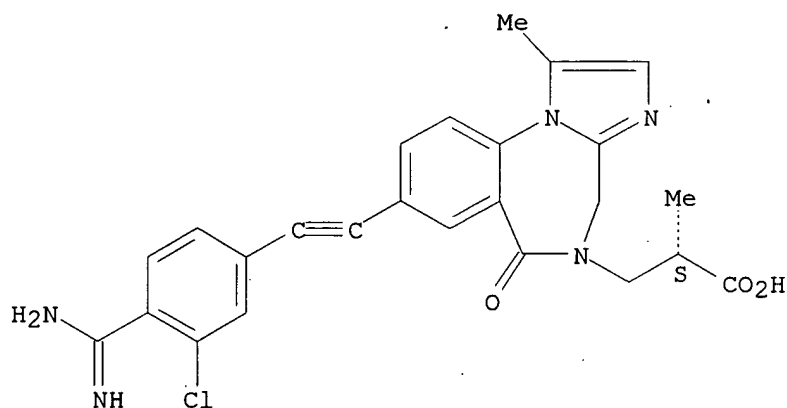


RN 167854-90-2 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-
, (S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

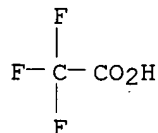
CRN 167854-89-9
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 167854-92-4 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-

09/868,356

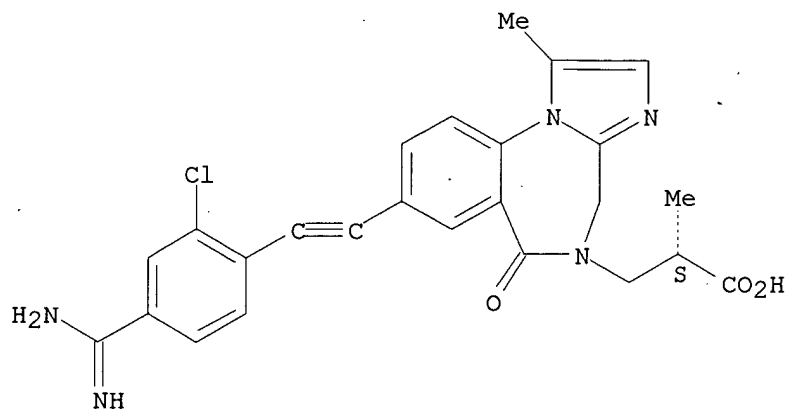
, (S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-91-3

CMF C25 H22 Cl N5 O3

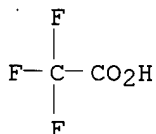
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-94-6 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.alpha.,1-dimethyl-6-oxo-,
(S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

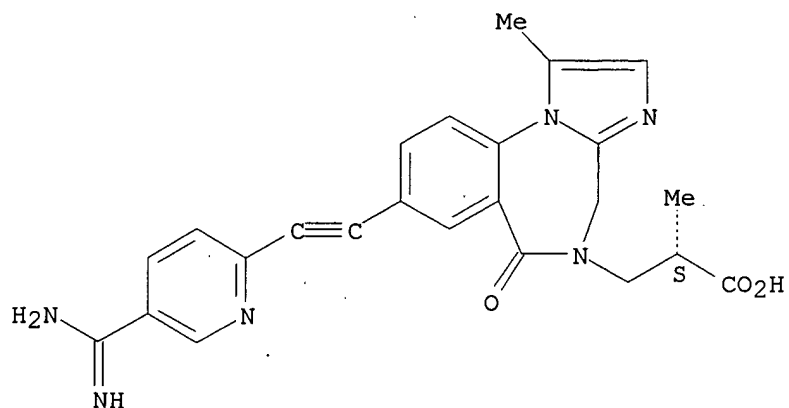
CM 1

CRN 167854-93-5

CMF C24 H22 N6 O3

Absolute stereochemistry.

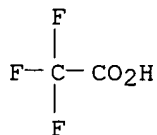
09/868,356



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 167854-96-8 CAPLUS

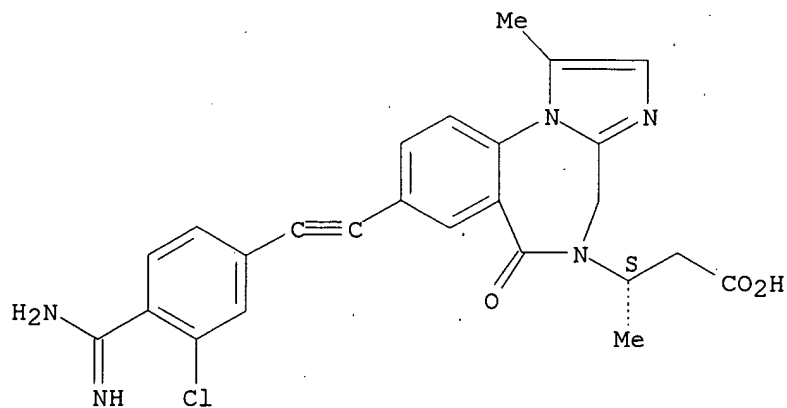
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)-3-chlorophenyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-95-7

CMF C25 H22 Cl N5 O3

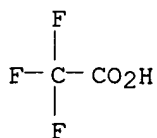
Absolute stereochemistry.



09/868,356

CM 2

CRN 76-05-1
CMF C2 H F3 O2

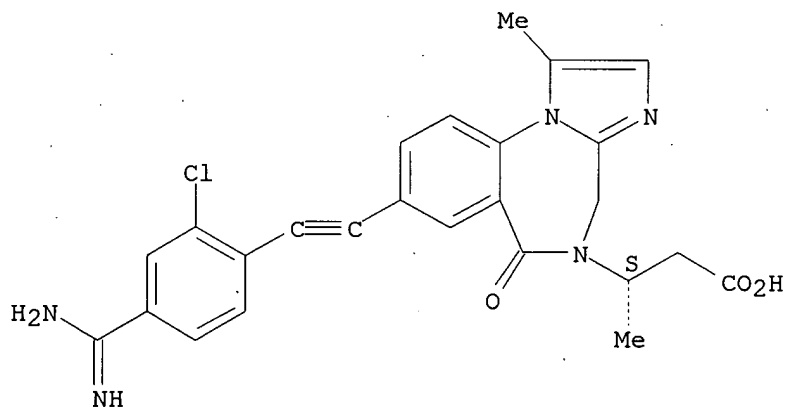


RN 167854-98-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[4-(aminoiminomethyl)-2-chlorophenyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

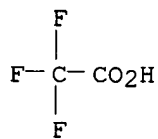
CRN 167854-97-9
CMF C25 H22 Cl N5 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 167855-00-7 CAPLUS

09/868,356

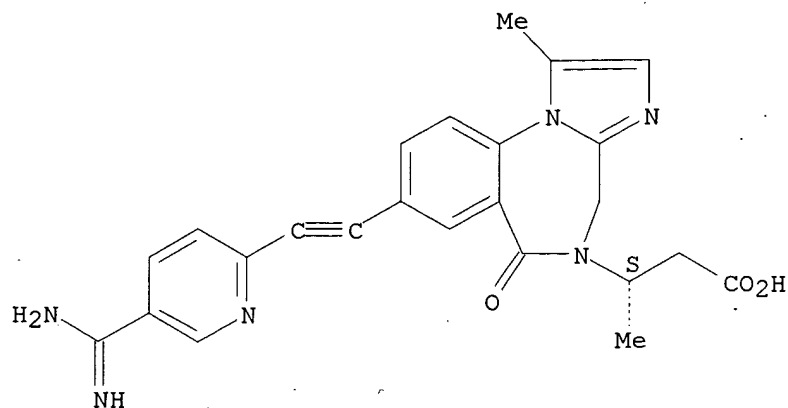
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[5-(aminoiminomethyl)-2-pyridinyl]ethynyl]-.beta.,1-dimethyl-6-oxo-,
(S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167854-99-1

CMF C24 H22 N6 O3

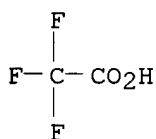
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 167853-81-8P 167853-83-0P 167855-32-5P
167855-44-9P 167855-45-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tricyclic benzodiazepinone inhibitors of the GPIIb/IIIa fibrinogen receptor which block blood platelet aggregation)

RN 167853-81-8 CAPLUS

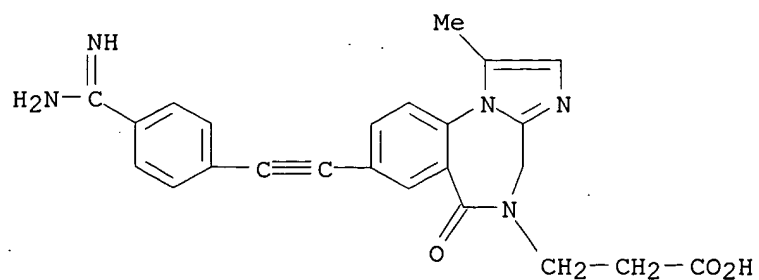
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, monoacetate (9CI)
(CA INDEX NAME)

CM 1

CRN 167853-80-7

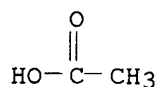
CMF C24 H21 N5 O3

09/868,356



CM 2

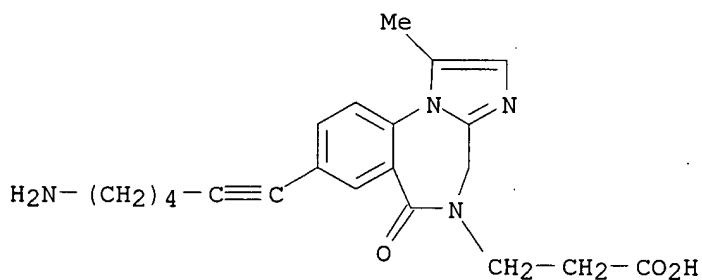
CRN 64-19-7
CMF C2 H4 O2



RN 167853-83-0 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-(6-amino-1-hexynyl)-1-methyl-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

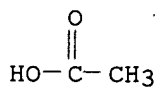
CM 1

CRN 167853-82-9
CMF C21 H24 N4 O3



CM 2

CRN 64-19-7
CMF C2 H4 O2

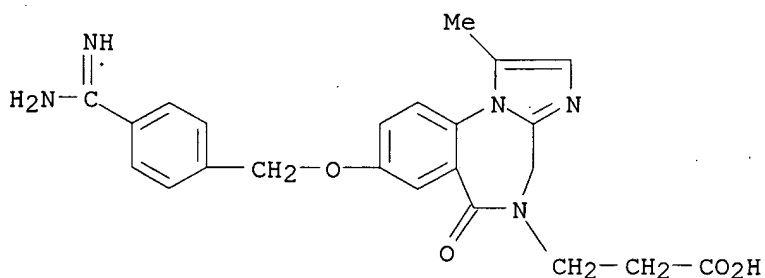


09/868,356

RN 167855-32-5 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]methoxy]-1-methyl-6-oxo-, monoacetate (9CI)
(CA INDEX NAME)

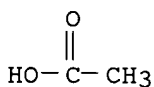
CM 1

CRN 167855-31-4
CMF C23 H23 N5 O4



CM 2

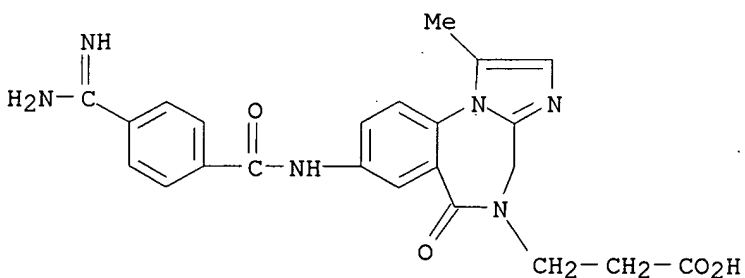
CRN 64-19-7
CMF C2 H4 O2



RN 167855-44-9 CAPLUS
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 167855-43-8
CMF C23 H22 N6 O4

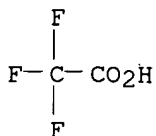


09/868,356

CM 2

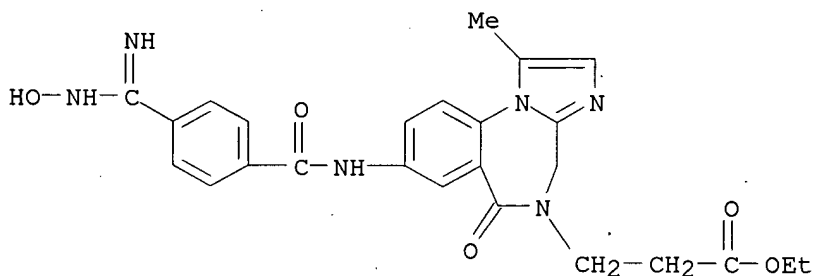
CRN 76-05-1

CMF C2 H F3 O2



RN 167855-45-0 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-[(hydroxyamino)iminomethyl]benzoyl]amino]-1-methyl-6-oxo-, ethyl
ester (9CI) (CA INDEX NAME)

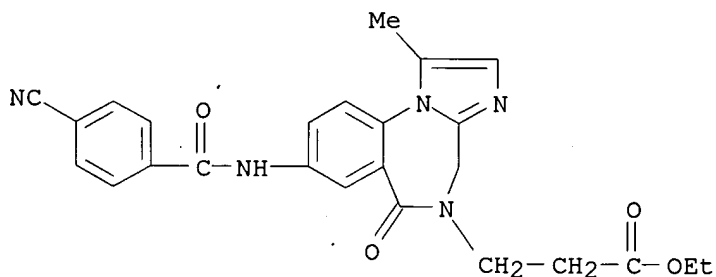


IT 167853-92-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of tricyclic benzodiazepinone inhibitors of the GPIIb/IIIa
fibrinogen receptor which block blood platelet aggregation)

RN 167853-92-1 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(4-cyanobenzoyl)amino]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
NAME)



IT 167853-94-3P 167853-96-5P 167853-97-6P

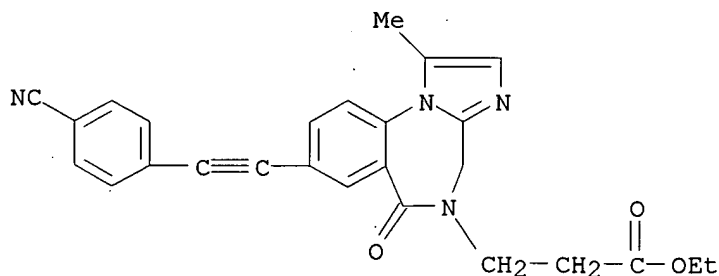
167854-00-4P 167854-14-0P 167854-16-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn. of tricyclic benzodiazepinone inhibitors of the GPIIb/IIIa
fibrinogen receptor which block blood platelet aggregation)

RN 167853-94-3 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[(4-cyanophenyl)ethynyl]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX
NAME)

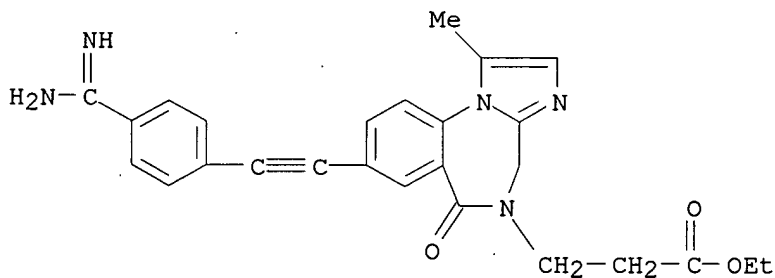
RN 167853-96-5 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,
8-[[4-(aminoiminomethyl)phenyl]ethynyl]-1-methyl-6-oxo-, ethyl ester,
monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 167853-95-4

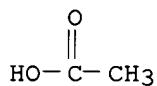
CMF C26 H25 N5 O3



CM 2

CRN 64-19-7

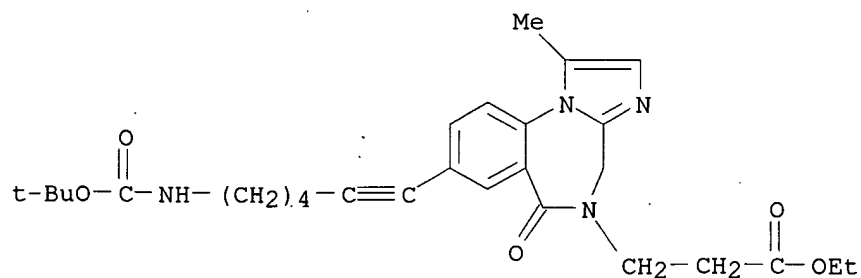
CMF C2 H4 O2



RN 167853-97-6 CAPLUS

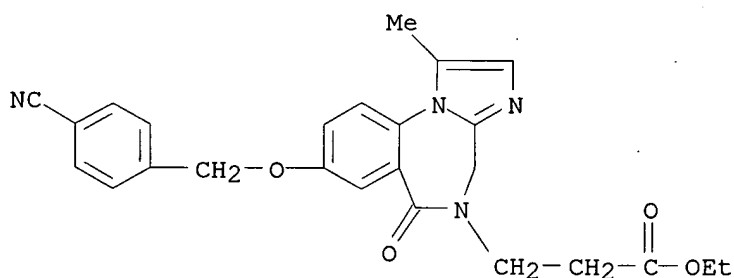
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid,

8-[6-[[(1,1-dimethylethoxy) carbonyl] amino]-1-hexynyl]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)



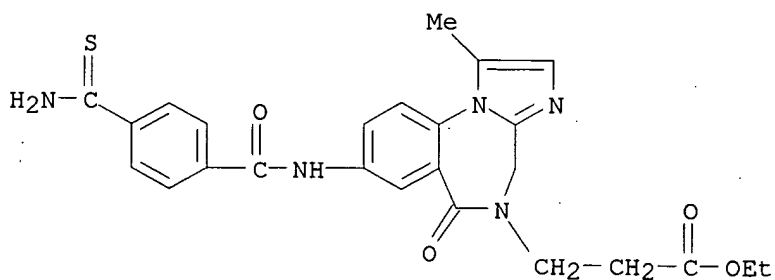
RN 167854-00-4 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[(4-cyanophenyl)methoxy]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 167854-14-0 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[[4-(aminothioxomethyl)benzoyl]amino]-1-methyl-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)



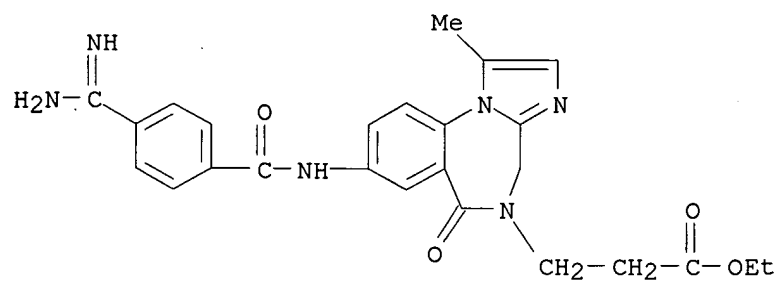
RN 167854-16-2 CAPLUS

CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-5(6H)-propanoic acid, 8-[[4-(aminoiminomethyl)benzoyl]amino]-1-methyl-6-oxo-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

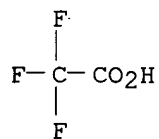
09/868,356

CRN 167854-15-1
CMF C25 H26 N6 O4

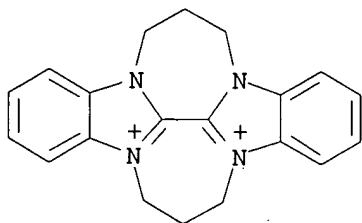


CM 2

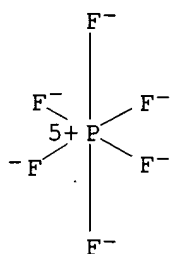
CRN 76-05-1
CMF C2 H F3 O2



~~LA~~ ANSWER 27 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1995:751102 CAPLUS
 DN 124:8776
 TI N,N'-Bridged Derivatives of 2,2'-Bibenzimidazole
 AU Shi, Zhiqiang; Thummel, Randolph P.
 CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
 SO Journal of Organic Chemistry (1995), 60(18), 5935-45
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 AB A series of 2,2'-bibenzimidazolium salts was prepd. by N,N'-bridging using dihaloalkanes. These salts may be reduced by either one or two electrons to the corresponding cation radical or neutral 2,2'-bibenzimidazolinylidene. The latter species undergoes a chemiluminescent reaction with dioxygen to afford conformationally unique ureaphanes. Two benzimidazole mols. may be joined by N,N'-bridges to form bis(benzimidazolium) salts which may be deprotonated with sodium hydride. Subsequent intramol. 2,2'-coupling leads to the same 2,2'-bibenzimidazolinylidenes. The structural features of the ureaphane oxidn. products have been studied by X-ray crystallog. and NMR. An equimolar mixt. of a 2,2'-bibenzimidazolium salt and the corresponding 2,2'-bibenzimidazolinylidene will coproportionate to form the analogous cation radical.
 IT **153652-55-2P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of bridged 2,2'-bibenzimidazolium salts)
 RN 153652-55-2 CAPLUS
 CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, bis[hexafluorophosphate(1-)] (9CI)
 (CA INDEX NAME)
 CM 1
 CRN 153652-54-1
 CMF C20 H20 N4



CM 2
 CRN 16919-18-9
 CMF F6 P
 CCI CCS

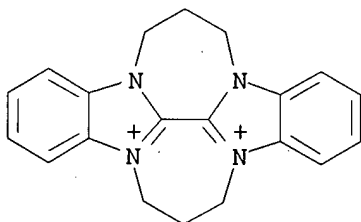


IT 153652-52-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of bridged 2,2'-bibenzimidazolium salts)

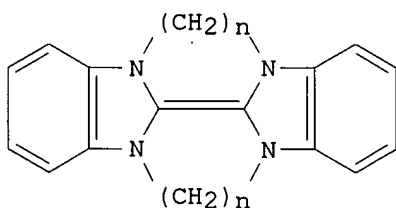
RN 153652-52-9 CAPLUS

CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-
kl]heptalene, 6,7,13,14-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



●2 Br⁻

~~DOI~~ ANSWER 28 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1995:515790 CAPLUS
 DN 123:228155
 TI Bridged dibenzimidazolinylienes as new derivatives of tetraaminoethylene
 AU Shi, Zhiqiang; Thummel, Randolph P.
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SO Tetrahedron Letters (1995), 36(16), 2741-4
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 OS CASREACT 123:228155
 GI



AB The deprotonation of N,N'-polymethylene bridged bis-benzimidazolium salts in the absence of air provides the corresponding bridged dibenzimidazolinylienes I ($n = 3, 4$), which undergo a spontaneous chemiluminescent reaction with dioxygen to afford ureaphanes.

IT 153652-55-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of bridged dibenzimidazolinylienes)

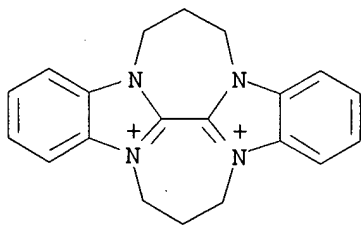
RN 153652-55-2 CAPLUS

CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, bis[hexafluorophosphate(1-)] (9CI)
 (CA INDEX NAME)

CM 1

CRN 153652-54-1

CMF C20 H20 N4

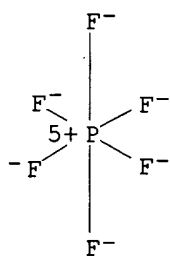


CM 2

CRN 16919-18-9

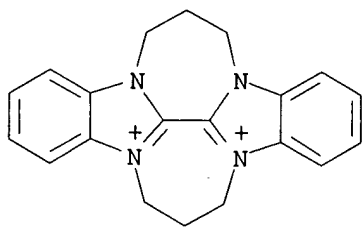
CMF F6 P

CCI CCS



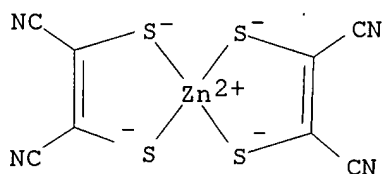
~~127~~ ANSWER 29 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1995:327241 CAPLUS
 DN 122:251827
 TI Charge-transfer complexes of metal dithiolenes. XV. Ion pair charge-transfer complexes of dithiolene metalates with diquaternary 2,2'-biimidazoles
 AU Lemke, Matthias; Knoch, Falk; Kisch, Horst; Salbeck, Josef
 CS Institut Anorganische Chemie, Universitaet Erlangen-Nuernberg, Erlangen, D-91058, Germany
 SO Chemische Berichte (1995), 128(2), 131-6
 CODEN: CHBEAM; ISSN: 0009-2940
 PB VCH
 DT Journal
 LA English
 AB Cycloalkylated biimidazolium dications (A2+) of redn. potential from -0.4 to -1.4 V form ion pair charge-transfer complexes {A2+[M(mnt)2]2-} with dithiolene metalates, M = Zn, Ni, Pd, Pt, mnt2- = maleonitrile-2,3-dithiolate. X-ray analyses of {P2BBIm2+[Ni(mnt)2]2-} [P2BBIm2+ = 1,1',3,3'-bis(propene-1,3-diyl)bibenzimidazolium] and {B2BIm2+[Pd(mnt)2]2-} [B2BIm2+ = 1,1',3,3'-bis(butane-1,4-diyl)biimidazolium] reveal that the solid-state structure is largely detd. by the geometry of the acceptor. When the latter is strongly twisted, the usually obsd. mixed donor-acceptor columns are modified to a chain-like arrangement. In the case of the bibenzimidazolium dication P2BBIm2+ the otherwise planar [Ni(mnt)2]2- becomes tetrahedrally distorted. By the application of the Hush model a reorganization energy of about 67 kJ/mol is estd. for the thermal electron transfer from [M(mnt)2]2- to A2+ when M = Ni, Pd, Pt, but considerable deviations from this model are obsd. when M = Zn. Irradn. of the free biimidazolium acceptors in the presence of EDTA affords the strongly reducing radical cations which reduce water to hydrogen in the presence of colloidal platinum. Attempts to sensitize this reaction by irradiating into the charge-transfer band of {A2+[M(mnt)2]2-} have failed until now. The molar absorptivity of one biimidazolium radical cation is measured by spectroelectrochem.
 IT 162477-52-3P 162477-53-4P 162477-54-5P
 162477-55-6P 162477-57-8P 162477-58-9P
 162477-60-3P 162477-61-4P 162477-62-5P
 162477-63-6P 162523-95-7P 162523-96-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chem., structure, and spectroscopy of ion pair CT complexes of dithiolene metalates with diquaternary biimidazoles)
 RN 162477-52-3 CAPLUS
 CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, (T-4)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-S,S']zincate(2-) (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 153652-54-1
 CMF C20 H20 N4

09/868,356



CM 2

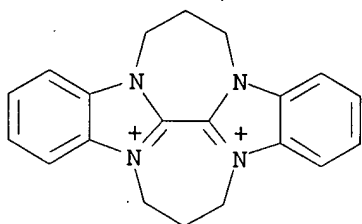
CRN 41139-14-4
CMF C8 N4 S4 Zn
CCI CCS



RN 162477-53-4 CAPLUS
CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-
kl]heptalene, 6,7,13,14-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-
butenedinitrilato(2-)-S,S']nickelate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

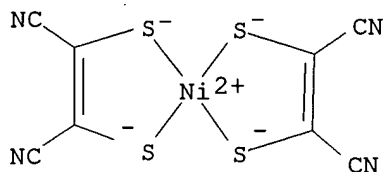
CRN 153652-54-1
CMF C20 H20 N4



CM 2

CRN 14876-79-0
CMF C8 N4 Ni S4
CCI CCS

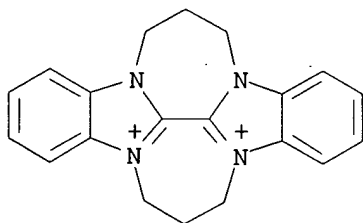
09/868,356.



RN 162477-54-5 CAPLUS
CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-
kl]heptalene, 6,7,13,14-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-
butenedinitrilato(2-)-S,S']palladate(2-) (1:1) (9CI) (CA INDEX NAME)

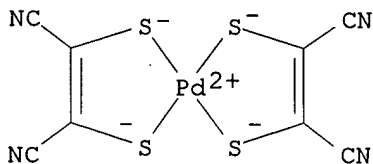
CM 1

CRN 153652-54-1
CMF C20 H20 N4



CM 2

CRN 19555-33-0
CMF C8 N4 Pd S4
CCI CCS

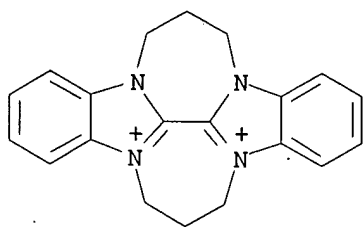


RN 162477-55-6 CAPLUS
CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-
kl]heptalene, 6,7,13,14-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-
butenedinitrilato(2-)-S,S']platinate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

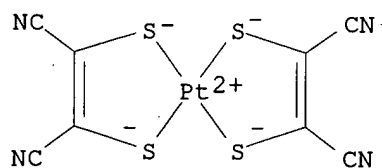
CRN 153652-54-1
CMF C20 H20 N4

09/868,356



CM 2

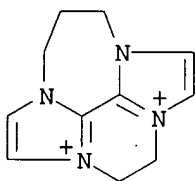
CRN 15152-99-5
CMF C8 N4 Pt S4
CCI CCS



RN 162477-57-8 CAPLUS
CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
3,4,8,9-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']palladate(2-) (1:1) (9CI) (CA INDEX NAME)

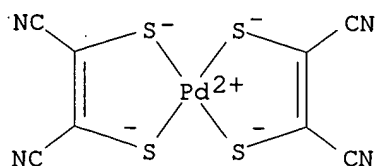
CM 1

CRN 162477-56-7
CMF C11 H14 N4



CM 2

CRN 19555-33-0
CMF C8 N4 Pd S4
CCI CCS



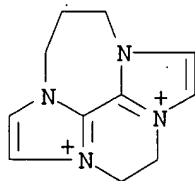
RN 162477-58-9 CAPLUS

CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
3,4,8,9-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']platinate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162477-56-7

CMF C11 H14 N4

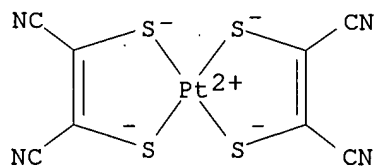


CM 2

CRN 15152-99-5

CMF C8 N4 Pt S4

CCI CCS



RN 162477-60-3 CAPLUS

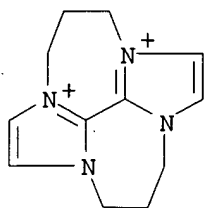
CN 1H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene,
4,5,9,10-tetrahydro-, (T-4)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']zincate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162477-59-0

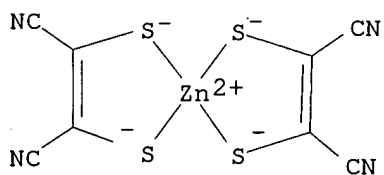
CMF C12 H16 N4

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CM 2

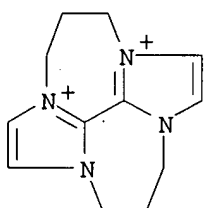
CRN 41139-14-4
CMF C8 N4 S4 Zn
CCI CCS



RN 162477-61-4 CAPLUS
CN 1H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene,
4,5,9,10-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']nickelate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

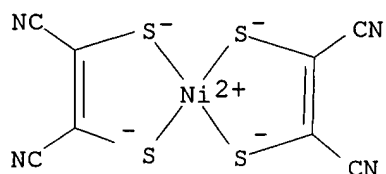
CRN 162477-59-0
CMF C12 H16 N4



CM 2

CRN 14876-79-0
CMF C8 N4 Ni S4
CCI CCS

09/868,356



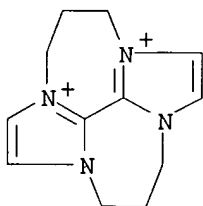
RN 162477-62-5 CAPLUS

CN 1H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene,
4,5,9,10-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']palladate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162477-59-0

CMF C12 H16 N4

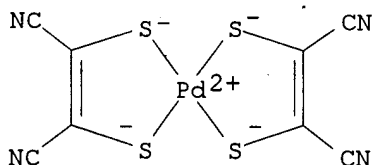


CM 2

CRN 19555-33-0

CMF C8 N4 Pd S4

CCI CCS



RN 162477-63-6 CAPLUS

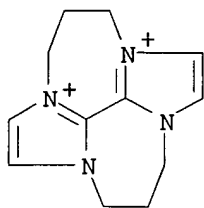
CN 1H,8H-7a,10a-Diaza-2a,5a-diazoniadicyclopenta[ef,kl]heptalene,
4,5,9,10-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']platinate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162477-59-0

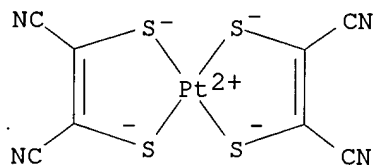
CMF C12 H16 N4

09/868,356



CM 2

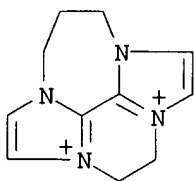
CRN 15152-99-5
CMF C8 N4 Pt S4
CCI CCS



RN 162523-95-7 CAPLUS
CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
3,4,8,9-tetrahydro-, (T-4)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']zincate(2-) (1:1) (9CI) (CA INDEX NAME)

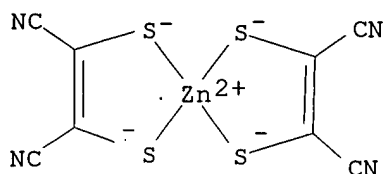
CM 1

CRN 162477-56-7
CMF C11 H14 N4



CM 2

CRN 41139-14-4
CMF C8 N4 S4 Zn
CCI CCS



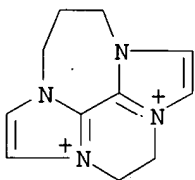
RN 162523-96-8 CAPLUS

CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
3,4,8,9-tetrahydro-, (SP-4-1)-bis[2,3-dimercapto-2-butenedinitrilato(2-)-
S,S']nickelate(2-) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 162477-56-7

CMF C11 H14 N4

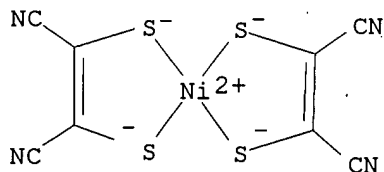


CM 2

CRN 14876-79-0

CMF C8 N4 Ni S4

CCI CCS



IT 120711-29-7

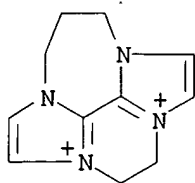
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)

(electron acceptor; chem., structure, and spectroscopy of ion pair CT
complexes of dithiolene metalates with diquaternary biimidazoles)

RN 120711-29-7 CAPLUS

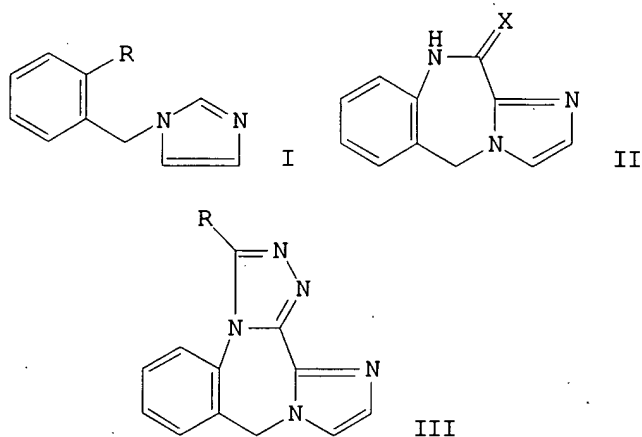
CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
3,4,8,9-tetrahydro-, dibromide (9CI) (CA INDEX NAME)

.09/868,356

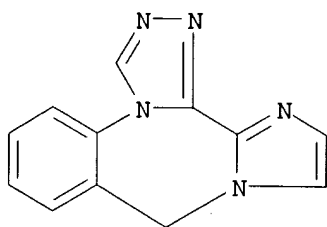


2 Br⁻

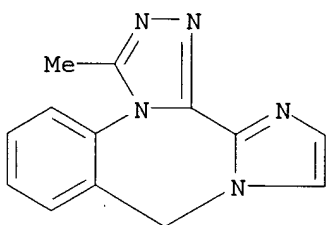
~~127~~ ANSWER 30 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1994:217596 CAPLUS
 DN 120:217596
 TI Research on nitrogen containing heterocyclic compounds. XIX. Synthesis of
 8H-imidazo[2,1-c]-s-triazolo[4,3-a][1,4]benzodiazepine and its
 1-derivatives
 AU Stefancich, Giorgio; Silvestri, Ramano; Artico, Marino
 CS Dip. Sci. Farm., Univ. Trieste, Trieste, 34127, Italy
 SO Journal of Heterocyclic Chemistry (1993), 30(2), 529-32
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 GI



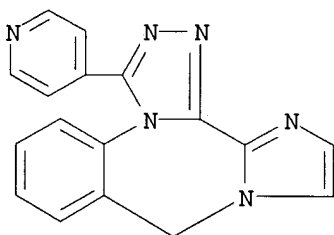
AB Reaction of 2-nitrobenzyl iodide with 1H-imidazole, in the presence of potassium tert-butoxide and 18-crown-6, gave 1-(2-nitrobenzyl)-1H-imidazole I (R = H). Trichloroacetylation of the latter gave trichloroacetylimidazole I (R = Cl₃CO), which on treatment with NaOEt was transformed into the corresponding ethoxycarbonyl deriv. I (R = CO₂Et). Redn. of the nitro group gave the corresponding amine, which was then cyclized to imidazobenzodiazepinone II (X = O). Treatment of lactam II with di-4-morpholinylphosphinic chloride followed by reaction of the intermediate II [X = H, OP(O)R₂ (R = 4-morpholinyl)] with RCONHNH₂ (R₂ = H, Me, 4-pyridinyl) gave the title compds. III.
 IT 153776-30-8P 153776-31-9P 153776-32-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 153776-30-8 CAPLUS
 CN 9H-Imidazo[2,1-c]-1,2,4-triazolo[4,3-a][1,4]benzodiazepine (9CI) (CA INDEX NAME)



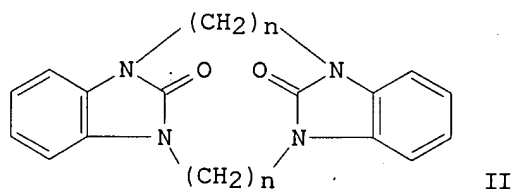
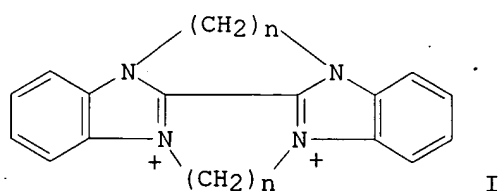
RN 153776-31-9 CAPLUS
 CN 9H-Imidazo[2,1-c]-1,2,4-triazolo[4,3-a][1,4]benzodiazepine, 3-methyl-
 (9CI) (CA INDEX NAME)



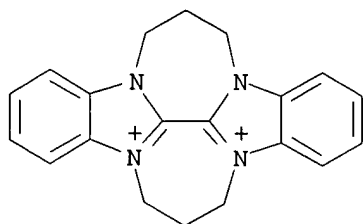
RN 153776-32-0 CAPLUS
 CN 9H-Imidazo[2,1-c]-1,2,4-triazolo[4,3-a][1,4]benzodiazepine,
 3-(4-pyridinyl)- (9CI) (CA INDEX NAME)



~~127~~ ANSWER 31 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1994:217434 CAPLUS
 DN 120:217434
 TI Bridged bibenzimidazolium salts and their conversion to ureaphanes
 AU Shi, Zhiqiang; Thummel, Randolph P.
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SO Tetrahedron Letters (1994), 35(1), 33-6
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 OS CASREACT 120:217434
 GI



AB The redn. of N,N'-polymethylene bridged 2,2'-bibenzimidazolium salts I ($n = 3, 4$) with tetrakis(dimethylamino)ethylene in air provides ureaphanes II (same n) whose conformations are dependent upon the length of the bridging chain.
 IT **153652-52-9P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reaction of, with hexafluorophosphate)
 RN 153652-52-9 CAPLUS
 CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



●2 Br⁻

IT 153652-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

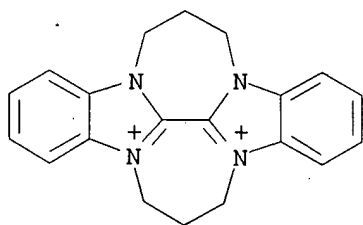
RN 153652-55-2 CAPLUS

CN 5H,12H-11b,14a-Diaza-4b,7a-diazoniadiindeno[1,2,3-ef:1',2',3'-kl]heptalene, 6,7,13,14-tetrahydro-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 153652-54-1

CMF C20 H20 N4

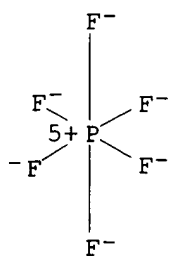


CM 2

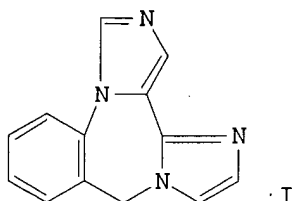
CRN 16919-18-9

CMF F6 P

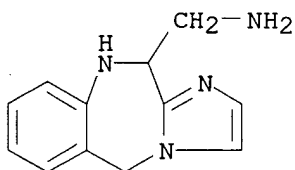
CCI CCS



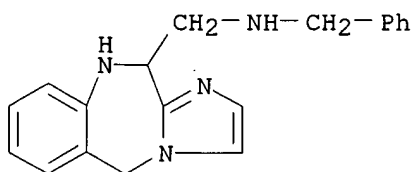
~~1~~7 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1992:469838 CAPLUS
 DN 117:69838
 TI Research on nitrogen containing heterocyclic compounds. XVII. Synthesis of 8H-diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine, a novel tetracyclic ring of pharmaceutical interest
 AU Stefancich, Giorgio; Artico, Marino; Silvestri, Romano
 CS Dip. Sci. Farm., Univ. Trieste, Trieste, 34127, Italy
 SO Journal of Heterocyclic Chemistry (1992), 29(2), 487-91
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 OS CASREACT 117:69838
 GI



AB The synthesis of 8H-diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine (I), a novel nitrogen-contg. tetracyclic ring, is reported starting from 5H-imidazo[2,1-c][1,4]benzodiazepine. Reaction of this compd. with MeNO₂ and subsequent redn. of the obtained nitromethyl deriv. afforded 11-(aminomethyl)-10,11-dihydro-5H-imidazo[2,1-c][1,4]benzodiazepine. Treatment of the latter compd. with HCHO led to 1,2,3,3a-tetrahydro-8H-diimidazo[1,5-a:2',1'-c]benzodiazepine, which was then oxidized to the title compd.
 IT **142427-61-0P 142427-67-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and cyclization of, with formaldehyde)
 RN 142427-61-0 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine-11-methanamine, 10,11-dihydro- (9CI)
 (CA INDEX NAME)



RN 142427-67-6 CAPLUS
 CN 5H-Imidazo[2,1-c][1,4]benzodiazepine-11-methanamine, 10,11-dihydro-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

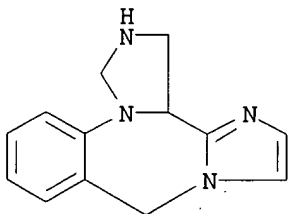


IT 142427-62-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydrogenation of)

RN 142427-62-1 CAPLUS

CN 8H-Diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine, 1,2,3,3a-tetrahydro- (9CI)
(CA INDEX NAME)



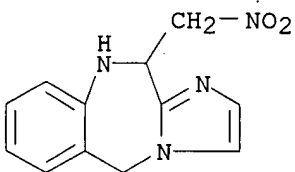
IT 142427-60-9P 142427-65-4P 142427-66-5P

142427-68-7P 142427-70-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenation of)

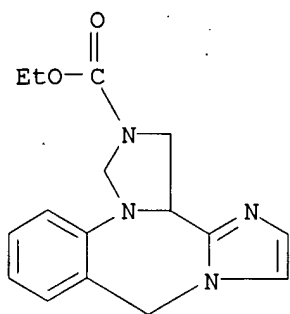
RN 142427-60-9 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine, 10,11-dihydro-11-(nitromethyl)- (9CI) (CA INDEX NAME)

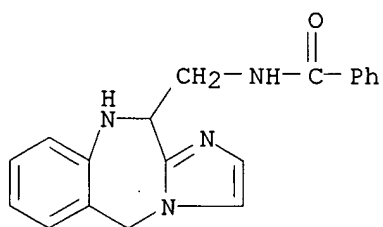


RN 142427-65-4 CAPLUS

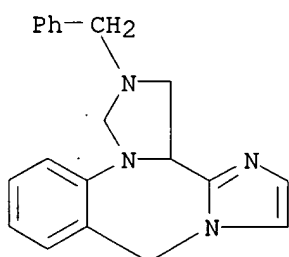
CN 8H-Diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine-2(1H)-carboxylic acid, 3,3a-dihydro-, ethyl ester (9CI) (CA INDEX NAME)



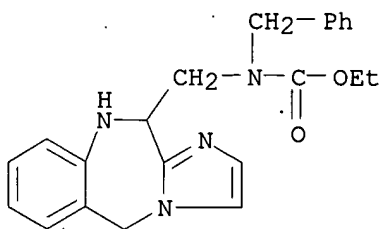
RN 142427-66-5 CAPLUS
 CN Benzamide, N-[(10,11-dihydro-5H-imidazo[2,1-c][1,4]benzodiazepin-11-yl)methyl]- (9CI) (CA INDEX NAME)



RN 142427-68-7 CAPLUS
 CN 8H-Diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine, 1,2,3,3a-tetrahydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 142427-70-1 CAPLUS
 CN Carbamic acid, [(10,11-dihydro-5H-imidazo[2,1-c][1,4]benzodiazepin-11-yl)methyl](phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

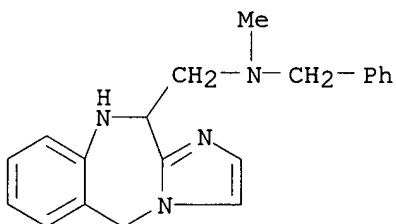


IT 142427-69-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)

RN 142427-69-8 CAPLUS

CN 5H-Imidazo[2,1-c][1,4]benzodiazepine-11-methanamine, 10,11-dihydro-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



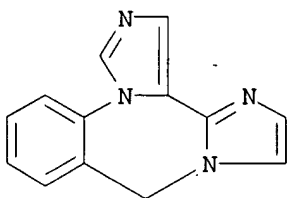
IT 142427-59-6P 142427-63-2P 142427-64-3P

142608-15-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 142427-59-6 CAPLUS

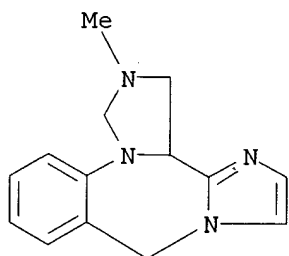
CN 8H-Diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine (9CI) (CA INDEX NAME)



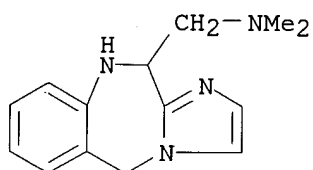
RN 142427-63-2 CAPLUS

CN 8H-Diimidazo[1,5-a:2',1'-c][1,4]benzodiazepine, 1,2,3,3a-tetrahydro-2-methyl- (9CI) (CA INDEX NAME)

09/868,356



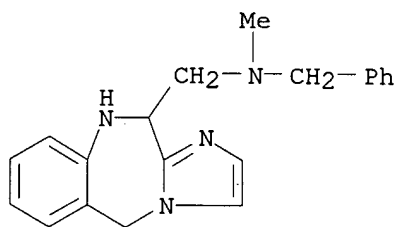
RN 142427-64-3 CAPLUS
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine-11-methanamine, 10,11-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 142608-15-9 CAPLUS
CN 5H-Imidazo[2,1-c][1,4]benzodiazepine-11-methanamine, 10,11-dihydro-N-methyl-N-(phenylmethyl)-; (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

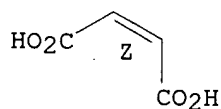
CRN 142427-69-8
CMF C20 H22 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



~~127~~ ANSWER 33 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1991:492239 CAPLUS

DN 115:92239

TI Synthesis and properties of new derivatives of 4,5-dicyanoimidazole and 4,4',5,5'-tetracyano-2,2'-biimidazole

AU Apen, Paul G.; Rasmussen, Paul G.

CS Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA

SO Journal of the American Chemical Society (1991), 113(16), 6178-87

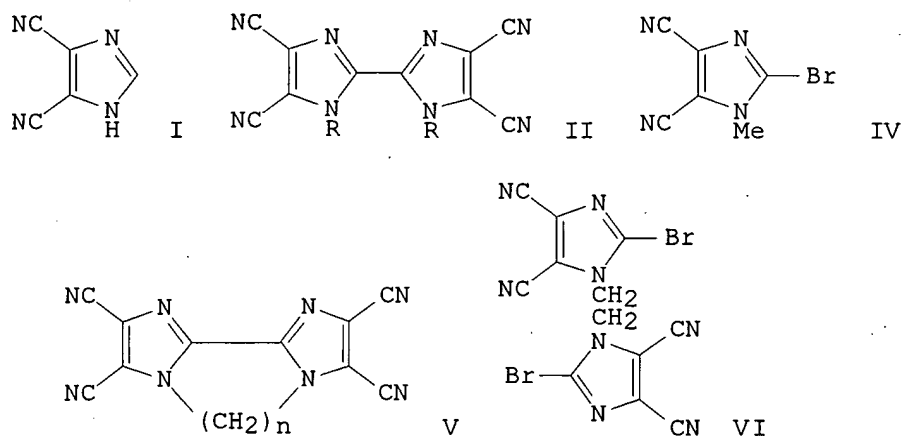
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CASREACT 115:92239

GI



AB The synthesis and properties of new derivs. of 4,5-dicyanoimidazole (I) and 4,4',5,5'-tetracyano-2,2'-biimidazole (II, R = H) (III) are reported. Conditions for selective metalation at the 2-position of N-protected 4,5-dicyanoimidazoles are described. Various protecting groups were used. Oxidative coupling of N-protected 2-lithio-4,5-dicyanoimidazoles with cupric chloride gives new 1,1'-disubstituted derivs. II (R = Me, CH₂OMe, CH₂Ph). Ullmann coupling of 1-methyl-2-bromo-4,5-dicyanoimidazole (IV) gives II (R = Me). Deprotection of II (R = Me or CH₂OMe) gives III, thus, several new routes to III are now available. Reaction of III with X(CH₂)_nX (X = Br, iodo; n = 2, 3, and 4) gives the corresponding 1,1'-alkyl-bridged derivs. V. V (n = 2) was also synthesized via an intramol. Ullmann coupling reaction of bis(bromodicyanoimidazolyl)ethane VI. The phys., structural, and electronic properties of these new cyanoimidazoles were investigated by using UV-visible spectroscopy and cyclic voltammetry. Dicyanoimidazoles and tetracyanobiimidazoles are moderate to weak electron acceptors. V (n = 2) forms a 1:1 complex with tetrathiafulvalene. The donor (D)-acceptor (A) complex, forms as red needles from acetonitrile soln. X-ray crystallog. of the complex showed extended alternate or mixed stacking (...DADADA...). The photoluminescence spectrum of the complex shows an emission band centered at 660 nm with onset of emission at 530 nm.

IT 134848-56-9P

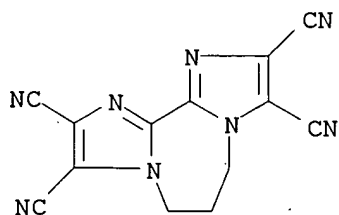
RL: SPN (Synthetic preparation); PREP (Preparation)

09/868,356

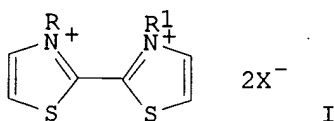
(prepn., UV-visible max., and cyclic voltammetry of)

RN 134848-56-9 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine-2,3,9,10-tetracarbonitrile,
6,7-dihydro- (9CI) (CA INDEX NAME)



~~127~~ ANSWER 34 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1990:478223 CAPLUS
 DN 113:78223
 TI Synthesis and properties of bridged 2,2'-bithiazolium salts
 AU Gouille, Veronique; Chirayil, Sara; Thummel, Randolph P.
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SO Tetrahedron Letters (1990), 31(11), 1539-42
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 OS CASREACT 113:78223
 GI



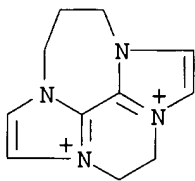
AB Bridged and methylated bithiazolium salts I [R = R1 = Me; RR1 = CH2CH2, (CH2)3, (CH2)4; X = PF6, iodo, BF4] were prepd. by alkylation of 2,2'-bithiazole. The electronic absorption spectra and redn. potentials were measured and stable radical cations of the di- and trimethylene bridged species were prepd.

IT 120711-29-7

RL: PRP (Properties)
 (redn. potential of)

RN 120711-29-7 CAPLUS

CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,
 3,4,8,9-tetrahydro-, dibromide (9CI) (CA INDEX NAME)



2 Br⁻

~~127~~ ANSWER 35 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1990:228635 CAPLUS

DN 112:228635

TI Ruthenium(II) complexes of N,N'-bridged derivatives of 2,2'-biimidazole

AU Gouille, Veronique; Thummel, Randolph P.

CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA

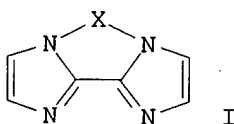
SO Inorganic Chemistry (1990), 29(9), 1767-72

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

GI



AB RuL₃[PF₆]₂ and RuL(bpy)₂[PF₆]₂ (L = I (X = (CH₂)_n (n = 2, 3, 4), o-CH₂C₆H₄CH₂), 2,2'-biimidazole; bpy = 2,2'-bipyridine) were prep'd. Mol. mechanics calcs. have been employed to compare the geometries of these ligands to those of analogous 2,2'-bipyridine systems. Anal. of ¹H NMR spectra indicates that in the coordinated state the bridged biimidazoles show greater conformational mobility than their bipyridine counterparts. For the dimethylene-bridged biimidazole, the bite angle is too unfavorable to allow bidentate coordination and NMR evidence points to monodentate coordination in the mixed-ligand complex. The electronic spectra of the RuL₃²⁺ complexes show absorption at approx. 400 nm, which indicates a high-lying π* state. This observation is reinforced by low oxidn. potentials and high redn. potentials for these systems. The mixed-ligand complexes show an absorption band at even shorter wavelength, which was assigned to the biimidazole metal-ligand charge transfer state. The redox chem. of these systems appears to be governed primarily by the bpy ligands.

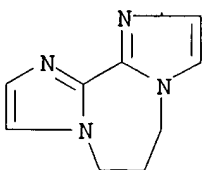
IT 54475-95-5

RL: PROC (Process)

(mol. dynamics and NMR of)

RN 54475-95-5 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



IT. 126949-43-7P 126949-47-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and electrochem. oxidn. and redn. and spectra of)

RN 126949-43-7 CAPLUS

CN Ruthenium(2+), tris(6,7-dihydro-5H-diimidazo[1,2-a:2',1'-c][1,4]diazepine-N1,N11)-, (OC-6-11)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

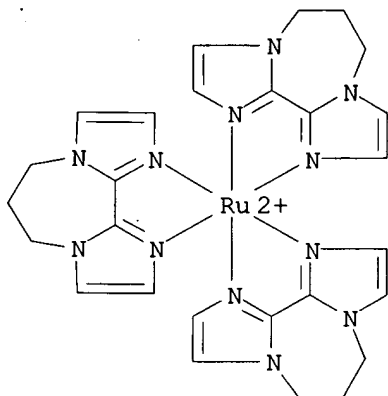
09/868,356

CM 1

CRN 126949-42-6

CMF C27 H30 N12 Ru

CCI CCS

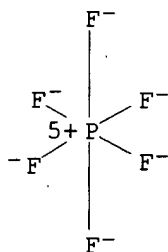


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



RN 126949-47-1 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-N,N')(6,7-dihydro-5H-diimidazo[1,2-a:2',1'-c][1,4]diazepine-N1,N11)-, (OC-6-32)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

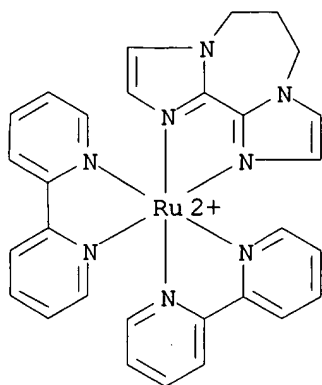
CM 1

CRN 126949-46-0

CMF C29 H26 N8 Ru

CCI CCS

09/868,356

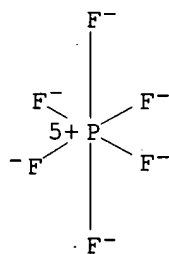


CM 2

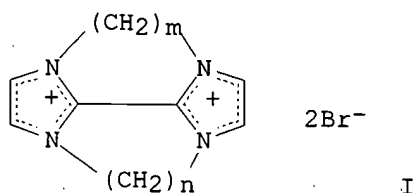
CRN 16919-18-9

CMF F6 P

CCI CCS



~~127~~ ANSWER 36 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN- 1989:423493 CAPLUS
 DN 111:23493
 TI Bridged derivatives of 2,2'-biimidazole
 AU Thummel, Randolph P.; Gouille, Veronique; Chen, Baili
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SO Journal of Organic Chemistry (1989), 54(13), 3057-61
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 OS CASREACT 111:23493
 GI



AB The reaction of 2,2'-biimidazole with 1,n-dihaloalkanes or o-xylylene dibromide leads to a series of N,N'-bridged derivs. When these substances are treated with a 2nd equiv. of 1,n-dihaloalkane, a series of bis-annulated biimidazolium salts, e.g., I ($m = 2$, $n = 3,4$; $m = n = 3,4$; $m = 3$, $n = 4$) were obtained. The conformations of these species are discussed with regard to their electronic absorption spectra and their 300-MHz 1H NMR spectra. The barriers for conformational inversion were lower than for the corresponding bis-annulated 2,2'-bipyridinium salts. The redox properties of these salts in MeCN and DMSO and their redns. become increasingly more difficult and less reversible as the system becomes less planar. These results are explained primarily based on the greater N,N'-distance in 2,2'-biimidazole as compared with 2,2'-bipyridine.

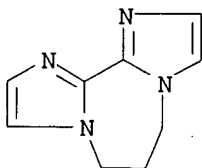
IT **54475-95-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and annulation of, with dihaloalkane, bridged biimidazole by)

RN 54475-95-5 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



IT **120711-29-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)

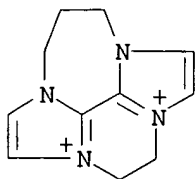
(prepn., conformation, and electrochem. redn. of)

RN 120711-29-7 CAPLUS

CN 7H-6a,9a-Diaza-2a,4a-diazoniacyclohept[jkl]-as-indacene,

09/868,356

3,4,8,9-tetrahydro-, dibromide (9CI) (CA INDEX NAME)


$$2 \text{ Br}^-$$

~~127~~ ANSWER 37 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1988:186776 CAPLUS
 DN 108:186776
 TI New 1,4-diazepines
 IN Harreus, Albrecht; Weber, Karl Heinz; Stransky, Werner; Walther, Gerhard; Muacevic, Gojko; Casals, Stenzel Jorge; Bechtel, Wolf Dietrich
 PA Boehringer Ingelheim K.-G., Fed. Rep. Ger.
 SO Ger. Offen., 31 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | DE 3610848 | A1 | 19871015 | DE 1986-3610848 | 19860401 |
| | DK 8701632 | A | 19871002 | DK 1987-1632 | 19870331 |
| | EP 240899 | A2 | 19871014 | EP 1987-104717 | 19870331 |
| | EP 240899 | A3 | 19890510 | | |
| | EP 240899 | B1 | 19920819 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | JP 62240686 | A2 | 19871021 | JP 1987-79533 | 19870331 |
| | AT 79622 | E | 19920915 | AT 1987-104717 | 19870331 |
| | CA 1314043 | A1 | 19930302 | CA 1987-533401 | 19870331 |
| | AU 8770955 | A1 | 19871008 | AU 1987-70955 | 19870401 |
| | AU 598526 | B2 | 19900628 | | |
| | IL 82084 | A1 | 19920329 | IL 1987-82084 | 19870401 |
| | US 5116971 | A | 19920526 | US 1990-584815 | 19900919 |
| PRAI | DE 1986-3610848 | | 19860401 | | |
| | EP 1987-104717 | | 19870331 | | |
| | US 1987-33966 | | 19870401 | | |

OS CASREACT 108:186776

GI For diagram(s), see printed CA Issue.

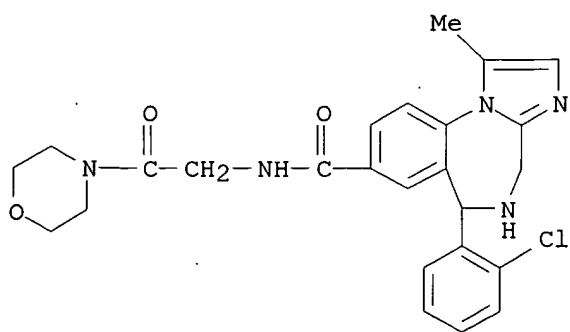
AB The title compds. [I and II; R1 = H, halo, (branched) C1-4 alkyl, cyclopropyl, C1-4 alkoxy; R2 = (substituted) Ph; R3 = H, (branched) alkyl; A = atoms to complete a Ph or thienyl ring substituted by an amino acid-contg. side chain; X = N, CH, CR4; R4 = halo] were prepd. as platelet activating factor antagonists (no data). 8-Carboxy-6-(2-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine (prepn. given) was stirred with 1,1'-carbonyldiimidazole in DMF/THF for 1 h at room temp and then glycine morpholide.HCl and Et3N were added. After 3d the mixt. was worked up to give N-[[1-methyl-6-(2-chlorophenyl)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepin-8-yl]carbonyl]glycine morpholide.

IT 113116-82-8P

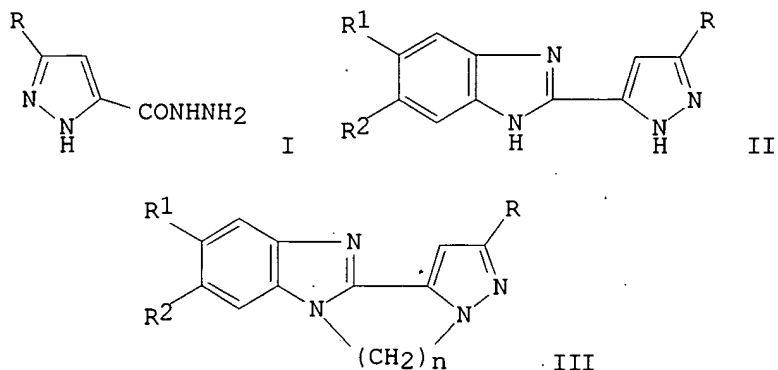
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as platelet activating factor antagonist)

RN 113116-82-8 CAPLUS

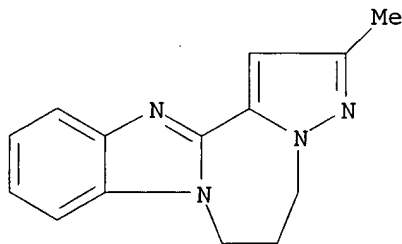
CN 4H-Imidazo[1,2-a][1,4]benzodiazepine-8-carboxamide, 6-(2-chlorophenyl)-5,6-dihydro-1-methyl-N-[2-(4-morpholinyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)



~~227~~ ANSWER 38 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1987:439769 CAPLUS
 DN 107:39769
 TI Synthesis and heterocyclization of 2-[3(5)pyrazolyl]benzimidazoles with phase-transfer catalysis
 AU Essassi, E. M.; Fifani, J.
 CS Lab. Chim. Org. Heterocycl., Fac. Sci., Rabat, Morocco
 SO Bulletin des Societes Chimiques Belges (1987), 96(1), 63-7
 CODEN: BSCBAG; ISSN: 0037-9646
 DT Journal
 LA French
 OS CASREACT 107:39769
 GI



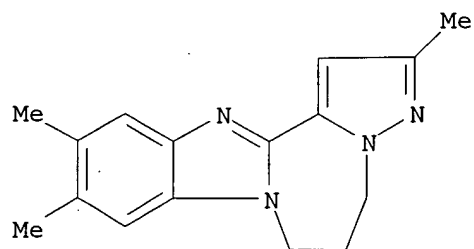
AB Fusion of o-diamines with pyrazolylhydrazides I (R = Me, Ph) gave pyrazolylbenzimidazoles II (R1 = H, Me, Cl, R2 = R1, NO2, CO2H). Treating II with Br(CH2)nBr (n = 2,3) under phase-transfer conditions gave benzimidazolopyrazolopyrazines (III; n = 2) and benzimidazolopyrazolodiazepines (III; n = 3).
 IT **109073-69-0P 109073-70-3P 109073-71-4P 109107-21-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 109073-69-0 CAPLUS
 CN 5H-Pyrazolo[5',1':3,4][1,4]diazepino[1,2-a]benzimidazole, 6,7-dihydro-2-methyl- (9CI) (CA INDEX NAME)



RN 109073-70-3 CAPLUS
 CN 5H-Pyrazolo[5',1':3,4][1,4]diazepino[1,2-a]benzimidazole,

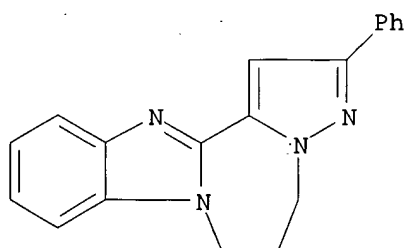
09/868,356

6,7-dihydro-2,10,11-trimethyl- (9CI) (CA INDEX NAME)



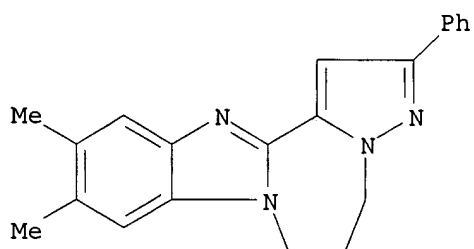
RN 109073-71-4 CAPLUS

CN 5H-Pyrazolo[5',1':3,4][1,4]diazepino[1,2-a]benzimidazole,
6,7-dihydro-2-phenyl- (9CI) (CA INDEX NAME)



RN 109107-21-3 CAPLUS

CN 5H-Pyrazolo[5',1':3,4][1,4]diazepino[1,2-a]benzimidazole,
6,7-dihydro-10,11-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



~~127~~ ANSWER 39 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1986:5852 CAPLUS

DN 104:5852

TI Synthesis of novel imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepines and pyrimido[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepines

AU Duceppe, Jean Simon; Gauthier, Jean

CS Dep. Chem., Ayerst Res. Lab., Montreal, QC, H3C 3J1, Can.

SO Journal of Heterocyclic Chemistry (1985), 22(2), 305-10

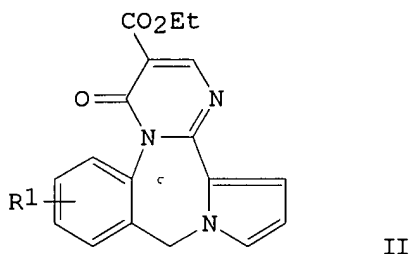
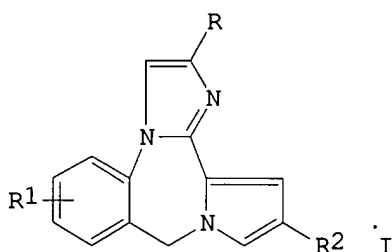
CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 104:5852

GI



AB Several 11-amino-5H-pyrrolo[2,1-c][1,4]benzodiazepines were condensed with $\text{BrCH}_2\text{COCO}_2\text{Et}$, $\text{H}_2\text{NCH}_2\text{CH}(\text{OMe})_2$, and $\text{EtOCH}:\text{C}(\text{CO}_2\text{Et})_2$ to yield 9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepines I ($\text{R} = \text{H}$, CO_2Et ; $\text{R}_1 = \text{H}$, Cl , Me ; $\text{R}_2 = \text{H}$, CHO) and 10H-pyrimido[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepines II. Several thioamides of I ($\text{R}_1 = \text{H}$; $\text{R}_2 = \text{CHO}$) were prepd. via Willgerodt-Kindler conditions.

IT 98156-71-9P 98156-72-0P 98156-73-1P

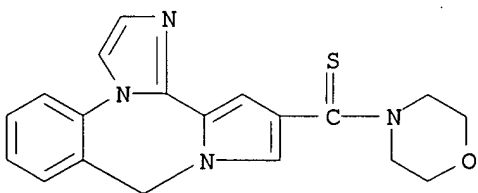
98156-74-2P 99390-39-3P 99390-40-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

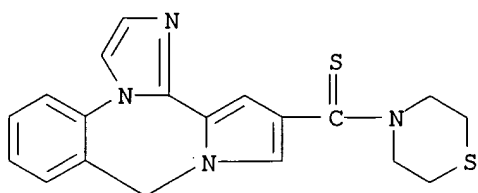
RN 98156-71-9 CAPLUS

CN Morpholine, 4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



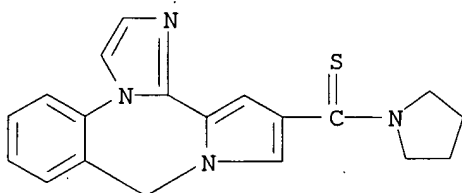
RN 98156-72-0 CAPLUS

CN Thiomorpholine, 4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



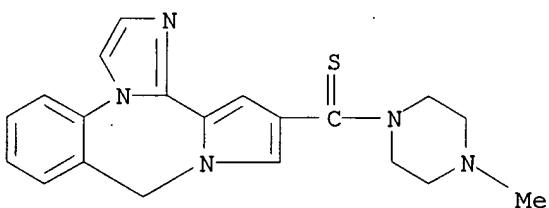
RN 98156-73-1 CAPLUS

CN Pyrrolidine, 1-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



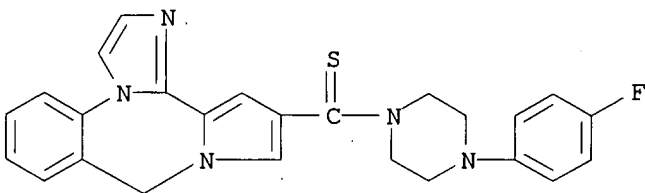
RN 98156-74-2 CAPLUS

CN Piperazine, 1-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)-4-methyl- (9CI) (CA INDEX NAME)



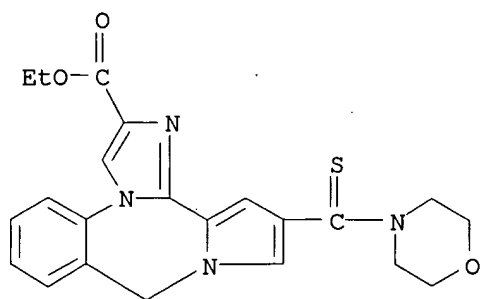
RN 99390-39-3 CAPLUS

CN Piperazine, 1-(4-fluorophenyl)-4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



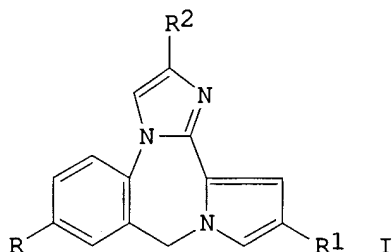
RN 99390-40-6 CAPLUS

CN 9H-Imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepine-2-carboxylic acid, 12-(4-morpholinylthioxomethyl)-, ethyl ester (9CI) (CA INDEX NAME)



~~127~~ ANSWER 40 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1985:523531 CAPLUS
 DN 103:123531
 TI Imidazo[2,1-a]pyrrolo[2,1-c][1,4]benzodiazepine derivatives, and their use
 IN Gauthier, Jean A.; Voith, Katherine; Asselin, Andre A.
 PA Ayerst, McKenna and Harrison, Inc., Can.
 SO U.S., 8 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---------------------|------|----------|-----------------|----------|
| PI | US 4521534 | A | 19850604 | US 1983-562905 | 19831219 |
| PRAI | US 1983-562905 | | 19831219 | | |
| OS | CASREACT 103:123531 | | | | |
| GI | | | | | |



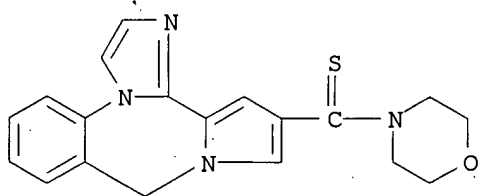
AB The title compds. I [R = H, halo, alkyl; R1 = H, CSR3 (R3 = morpholino, pyrrolidino, piperidino, 4-alkylpiperazino, 4-(4-fluorophenyl)piperazino); R2 = H, alkoxy-carbonyl] and their addn. salts were prepd. as antiobesity agents. Thus, 11-amino-5H-pyrrolo[2,1-c][1,4]benzodiazepine was treated with H2NCH2CH(OMe)2 to give [(5H-pyrrolo[2,1-c][1,4]benzodiazepin-11-yl)amino]acetaldehyde, which was cyclized by HCl to give I (R = R1 = R2 = H) (II). At 30 mg/kg II decreased the food intake in rats by 51%.

IT **98156-71-9P 98156-72-0P 98156-73-1P**
98156-74-2P 98156-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and appetite depressant activity of)

RN 98156-71-9 CAPLUS

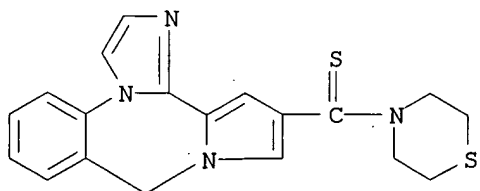
CN Morpholine, 4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



RN 98156-72-0 CAPLUS

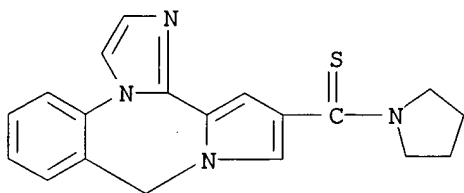
CN Thiomorpholine, 4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-

ylthioxomethyl)- (9CI) (CA INDEX NAME)



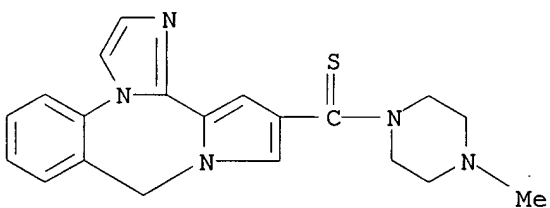
RN 98156-73-1 CAPLUS

CN Pyrrolidine, 1-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)- (9CI) (CA INDEX NAME)



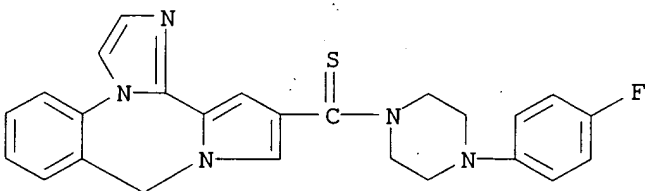
RN 98156-74-2 CAPLUS

CN Piperazine, 1-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)-4-methyl- (9CI) (CA INDEX NAME)



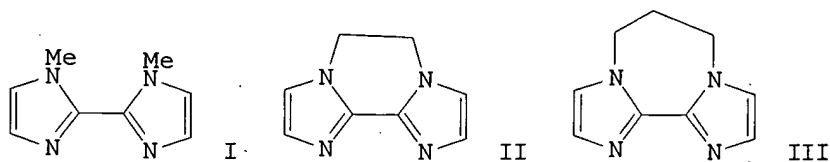
RN 98156-75-3 CAPLUS

CN Piperazine, 1-(4-fluorophenyl)-4-(9H-imidazo[1,2-a]pyrrolo[2,1-c][1,4]benzodiazepin-12-ylthioxomethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



3 HCl

~~DO7~~ ANSWER 41 OF 46 CAPLUS COPYRIGHT 2003 ACS
~~AN~~ 1982:161809 CAPLUS
 DN 96:161809
 TI Lone-pair cooperativity in the N-alkylation of some derivatives
 2,2'-biimidazole
 AU Deady, Leslie W.
 CS Org. Chem. Dep., La Trobe Univ., Bundoora, 3083, Australia
 SO Australian Journal of Chemistry (1981), 34(12), 2569-76
 CODEN: AJCHAS; ISSN: 0004-9425
 DT Journal
 LA English
 GI



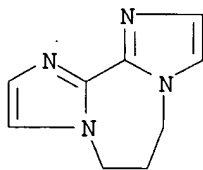
AB The relative rates of N-alkylation of I, II, and III with a variety of alkylating agents are reported. Irresp. of the alkylating agent, the order of reactivity was III (where the biimidazole has an addnl. three-carbon bridge) > II (two-carbon bridge) > I (no bridge), with a max. of 317:1 I-III for reaction with MeOCH₂Cl. These results support the idea of N atom lone-pair cooperativity in the alkylation reactions. Variation in the rate ratios with changes in alkylating agent are discussed.

IT **81416-11-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 81416-11-7 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

IT **54475-95-5**

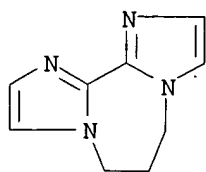
RL: RCT (Reactant); RACT (Reactant or reagent)

(N-alkylation of, kinetics of, nitrogen atom lone-pair cooperativity and)

RN 54475-95-5 CAPLUS

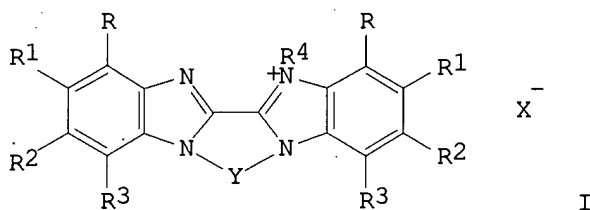
CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)

09/868,356



127 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1981:463696 CAPLUS
 DN 95:63696
 TI Quaternized bridged benzimidazolyl benzimidazoles and their use
 IN Schoenberger, Norbert; Schinzel, Erich; Martini, Thomas; Roesch, Guenther
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 23 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---------------------------|------|----------|-----------------|----------|
| PI | DE 2939916 | A1 | 19810423 | DE 1979-2939916 | 19791002 |
| | EP 27897 | A1 | 19810506 | EP 1980-105767 | 19800925 |
| | R: CH, DE, FR, GB, IT, NL | | | | |
| | US 4309551 | A | 19820105 | US 1980-191709 | 19800929 |
| | JP 56057851 | A2 | 19810520 | JP 1980-135930 | 19801001 |
| PRAI | DE 1979-2939916 | | 19791002 | | |
| GI | | | | | |



AB Title compds. having the general structure I are prepd., where R-R3 = H or a substituent, or any two adjacent R groups taken together may form a fused benzene ring; R4 = alkyl or substituted alkyl; Y = (CH2)_n (n = 1-4) or (CR₂₅)₁₋₃ (R₅ = alkyl or phenyl); and X⁻ = halide, alkylsulfonate, etc. I are esp. useful as fluorescent whiteners for acrylic fibers. Thus, quaternization of 1,1'-dimethylene-5,5',6,6'-tetramethyl-2,2'-bibenzimidazole [78196-62-0] (from 5,5',6,6'-tetramethyl-2,2'-bibenzimidazole [14468-52-1] and 1,2-dibromoethane [106-93-4]) with Me₂SO₄ in DMF at 80-120.degree. gave pale yellow cryst. I (R = R3 = H, R1 = R2 = R4 = Me, Y = CH₂CH₂, X = MeSO₄) [78196-76-6] showing a blue-violet fluorescence in H₂O or DMF and fluorescent whitening properties on acrylic fibers. The corresponding compd. in which the CH₂CH₂ bridge was replaced by two Me groups showed no whitening effect.

IT **78196-66-4P**

RL: PREP (Preparation)

(manuf. of, as a fluorescent brightener for acrylic fibers)

RN 78196-66-4 CAPLUS

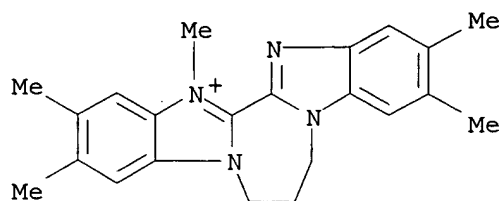
CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepinium, 7,8-dihydro-2,3,11,12,14-pentamethyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 78196-65-3

CMF C22 H25 N4

09/868,356



CM 2

CRN 21228-90-0

CMF C H3 O4 S

$$\text{Me}-\text{O}-\text{SO}_3^-$$

IT 78196-67-5P

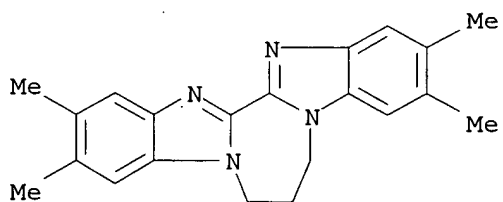
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

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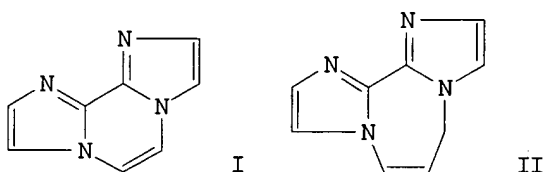

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RN 78196-67-5 CAPLUS

CN 6H-Bisbenzimidazo[1,2-a:2',1'-c][1,4]diazepine, 7,8-dihydro-2,3,11,12-tetramethyl- (9CI) (CA INDEX NAME)



~~LN~~ 7 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1976:144589 CAPLUS
 DN 84:144589
 TI New antiprotozoal agents
 AU Melloni, Piero; Fusar-Bassini, Domenico; Logemann, Willy; Forgione, Angelo; Dradi, Emanuele; De Carneri, Ivo; Bianchi, Alberta; Trane, Franca
 CS Carlo Erba Res. Inst., Milan, Italy
 SO European Journal of Medicinal Chemistry (1975), 10(5), 514-18
 CODEN: EJMCA5; ISSN: 0223-5234
 DT Journal
 LA English
 GI



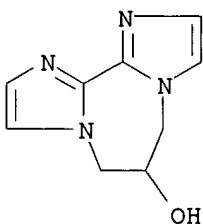
AB Of the 19 nitroderivs. of diimidazo-[1,2-a; 2',1'-c]-pyrazine (I) and diimidazo-[1,2-a; 2',1'-c][1,4]-diazepine (II) tested against *Trichomonas vaginalis*, *Entamoeba histolytica* and *Giardia muris*, some of the compds. displayed in vitro and in vivo (with mice and rats) activities several times higher than metronidazole [443-48-1]. The prepn. of the nitroderivs. of I and II is described. For the compds. to be active, the nitro group had to be in the ortho position to the pyrrolic type nitrogen. The I derivs. were more active than the corresponding II derivs., and the 5,6-dihydro derivs. were slightly more active than the corresponding 5,6-unsatd. compds.

IT **54475-99-9**

RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation and pivaloylation and nitration of)

RN 54475-99-9 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro- (9CI) (CA INDEX NAME)



IT **54475-95-5**

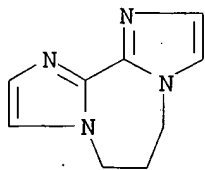
RL: RCT (Reactant); RACT (Reactant or reagent)
 (nitration of)

RN 54475-95-5 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)

09/868,356

NAME)



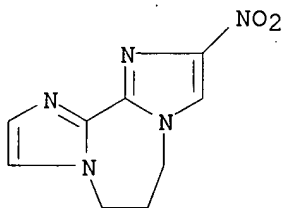
IT 57831-72-8P 57831-73-9P 57831-75-1P

57831-76-2P 57831-77-3P 57831-78-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and protozoacidal activity of)

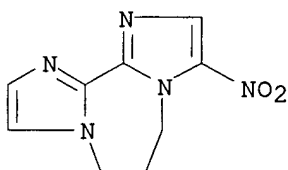
RN 57831-72-8 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro-2-nitro- (9CI) (CA
INDEX NAME)



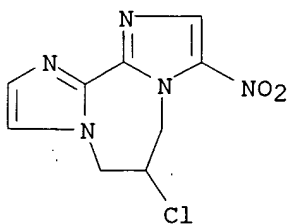
RN 57831-73-9 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro-3-nitro- (9CI) (CA
INDEX NAME)



RN 57831-75-1 CAPLUS

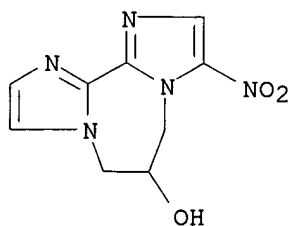
CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6-chloro-6,7-dihydro-3-nitro-
(9CI) (CA INDEX NAME)



RN 57831-76-2 CAPLUS

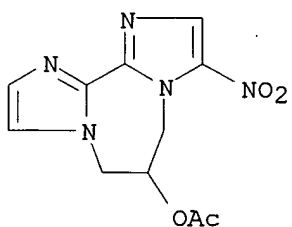
09/868,356

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro-3-nitro- (9CI)
(CA INDEX NAME)



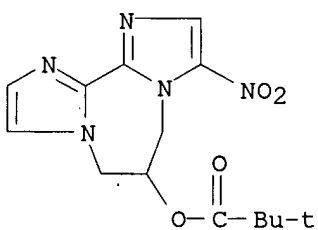
RN 57831-77-3 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro-3-nitro-,
acetate (ester) (9CI) (CA INDEX NAME)

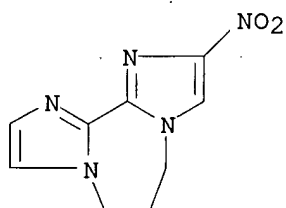


RN 57831-78-4 CAPLUS

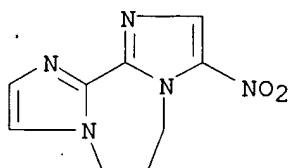
CN Propanoic acid, 2,2-dimethyl-, 6,7-dihydro-3-nitro-5H-diimidazo[1,2-
a:2',1'-c][1,4]diazepin-6-yl ester (9CI) (CA INDEX NAME)



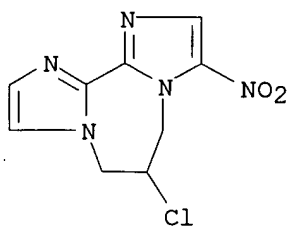
~~L27~~ ANSWER 44 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1976:39353 CAPLUS
 DN 84:39353
 TI Diimidazopirazines and diimidazodiazepines, a new class of heterocycles with antiprotozoan activity
 AU Melloni, P.; Logemann, W.; Dradi, E.; Confalonieri, C.; Trane, F.; De Carneri, I.
 CS Carlo Erba Res. Inst., Milan, Italy
 SO Prog. Chemother. (Antibacterial, Antiviral, Antineoplast.), Proc. Int. Congr. Chemother., 8th (1974), Meeting Date 1973, Volume 1, 983-7.
 Editor(s): Daikos, George K. Publisher: Hell. Soc. Chemother., Athens, Greece.
 CODEN: 31TFAO
 DT Conference
 LA English
 AB Derivs. of diimidazo[1,2-a; 2,1-c]pirazine [54475-96-6] and diimidazo[1,2-a; 2,1-c]diazepine[1,4] [54475-97-7] were prepd. and subjected to uv and ir spectral anal. for structure detn. The compds. contg. a nitro group at position 3 were comparable to metronidazole [443-48-1] in their ability to inhibit Trichomonas vaginalis and Entamoeba histolytica in vivo and in vitro.
 IT **57831-72-8 57831-73-9 57831-75-1**
57831-76-2 57831-77-3 57831-78-4
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (protozoacidal activity of)
 RN 57831-72-8 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro-2-nitro- (9CI) (CA INDEX NAME)



RN 57831-73-9 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro-3-nitro- (9CI) (CA INDEX NAME)

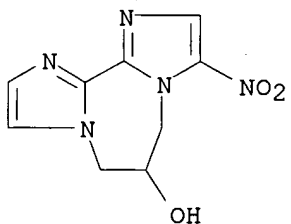


RN 57831-75-1 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6-chloro-6,7-dihydro-3-nitro- (9CI) (CA INDEX NAME)



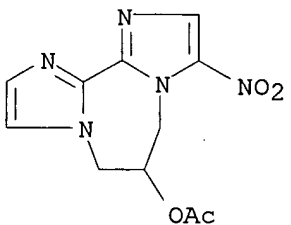
RN 57831-76-2 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro-3-nitro- (9CI)
(CA INDEX NAME)



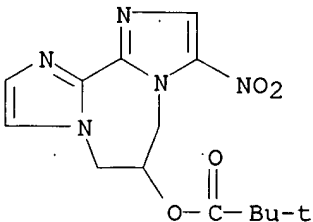
RN 57831-77-3 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro-3-nitro-,
acetate (ester) (9CI) (CA INDEX NAME)

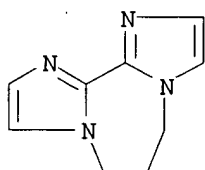


RN 57831-78-4 CAPLUS

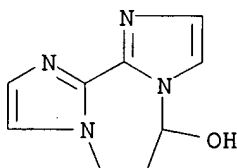
CN Propanoic acid, 2,2-dimethyl-, 6,7-dihydro-3-nitro-5H-diimidazo[1,2-
a:2',1'-c][1,4]diazepin-6-yl ester (9CI) (CA INDEX NAME)



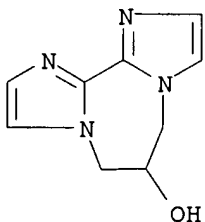
~~17~~ ANSWER 45 OF 46 CAPLUS COPYRIGHT 2003 ACS
 AN 1975:43375 CAPLUS
 DN 82:43375
 TI Synthesis of diimidazo[1,2-a:2',1'-c]pyrazines and diimidazo[1,2-a:2',1'-c][1,4]diazepines
 AU Melloni, P.; Fasar-Bassini, D.; Dradi, E.; Confalonieri, C.
 CS Dep. Chem., Carlo Erba Res. Inst., Milan, Italy
 SO Journal of Heterocyclic Chemistry (1974), 11(5), 731-5
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 AB The diimidazo[1,2-a:2',1'-c]pyrazine and 5H-diimidazo[1,2-a:2',1'-c][1,4]diazepine ring systems were prepd. from 2,2'-biimidazole.
 IT 54475-95-5P 54475-98-8P 54475-99-9P
 54476-00-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 54475-95-5 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



RN 54475-98-8 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-5-ol, 6,7-dihydro- (9CI) (CA INDEX NAME)



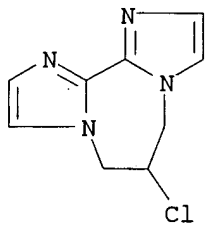
RN 54475-99-9 CAPLUS
 CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepin-6-ol, 6,7-dihydro- (9CI) (CA INDEX NAME)



09/868,356

RN 54476-00-5 CAPLUS

CN 5H-Diimidazo[1,2-a:2',1'-c][1,4]diazepine, 6-chloro-6,7-dihydro- (9CI)
(CA INDEX NAME)



~~127~~ ANSWER 46 OF 46 CAPLUS COPYRIGHT 2003 ACS

AN 1971:510235 CAPLUS

DN 75:110235

TI Reaction of 2-(4-thiazolyl)benzimidazole (thiabendazole) with alkyl halides

AU Maynard, Judith A.; Rae, I. D.; Rash, D.; Swan, J. M.

CS Dep. Chem., Monash Univ., Clayton, Australia

SO Australian Journal of Chemistry (1971), 24(9), 1873-81

CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

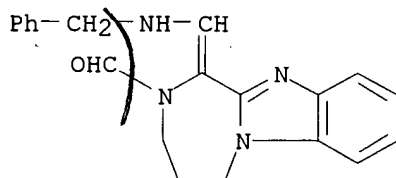
AB 2-(4-Thiazolyl)benzimidazole (thiabendazole) is alkylated at a benzimidazole N by reaction with NaH and an alkyl halide. With 1,3-dibromopropane and 1,2-dibromoethane, the thiazole N is also alkylated to give quaternary salts contg. the 6,7-dihydro-5H-thiazolo[3',4'.1,2][1,4]diazepino[8,9-a]benzimidazole and 5,6-dihydrothiazolo[3,'4'.1,2]pyrazino[7,8-a]benzimidazole ring systems, resp. The structures proposed for these tetracyclic products are supported by spectroscopic examn. of the products formed by alkali fission of their thiazole rings.

IT 33705-50-9P 33813-39-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

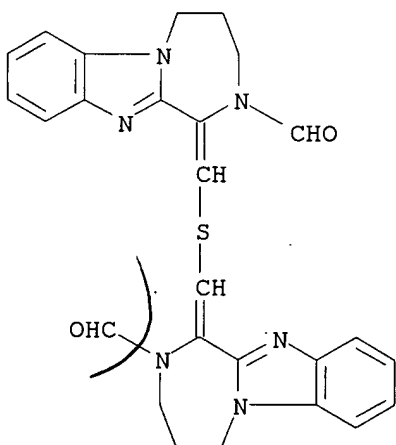
RN 33705-50-9 CAPLUS

CN 1H-[1,4]Diazepino[1,2-a]benzimidazole-2(3H)-carboxaldehyde,
1-[(benzylamino)methylene]-4,5-dihydro- (8CI) (CA INDEX NAME)



RN 33813-39-7 CAPLUS

CN 1H-[1,4]Diazepino[1,2-a]benzimidazole-2(3H)-carboxaldehyde,
1,1'-(thiodimethylidyne)bis[4,5-dihydro- (8CI) (CA INDEX NAME)



09/868,356